



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:19 PM UTC

PDB ID : 4HYC / pdb_00004hyc
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

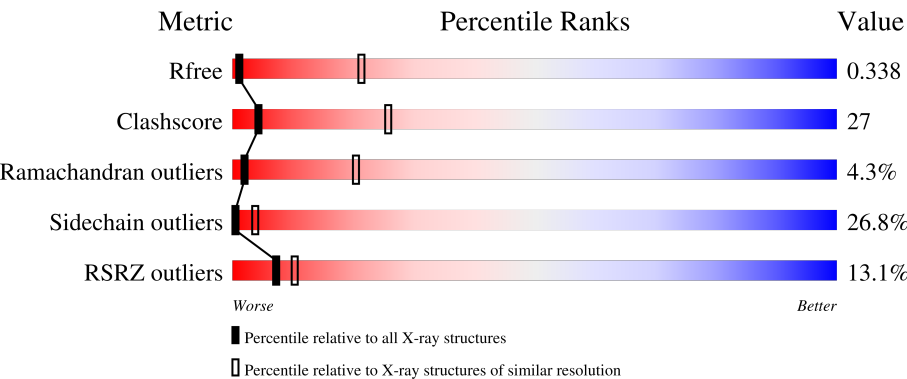
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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 $\leq 5\%$. 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	8% 34% 36% 11% • 18%
1	B	301	11% 35% 34% 13% 18%
1	C	301	10% 36% 35% 11% 18%
1	D	301	8% 31% 39% 11% 18%
1	E	301	12% 37% 32% 12% • 18%

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Mol	Chain	Length	Quality of chain
1	F	301	12% 32% 36% 13% 18%
1	G	301	13% 31% 37% 14% 18%
1	H	301	12% 35% 34% 12% 18%

2 Entry composition

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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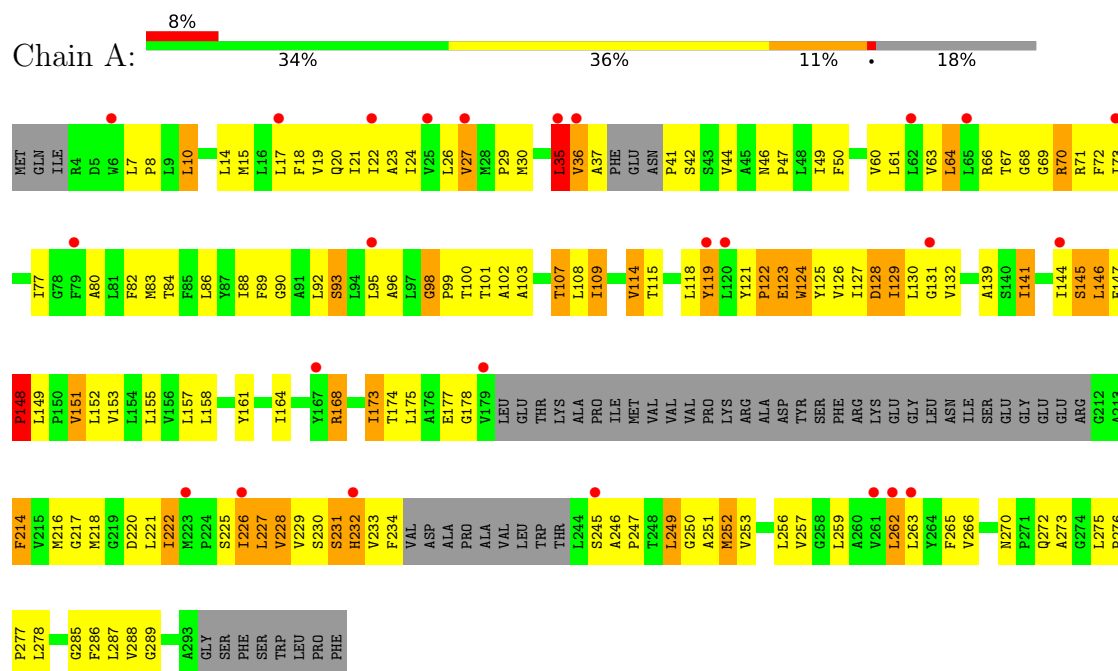
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Chain	Residue	Modelled	Actual	Comment	Reference
C	148	PRO	VAL	engineered mutation	UNP A3CWV0
C	229	VAL	ALA	engineered mutation	UNP A3CWV0
D	40	ASN	ASP	engineered mutation	UNP A3CWV0
D	42	SER	GLU	engineered mutation	UNP A3CWV0
D	147	GLU	ALA	engineered 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

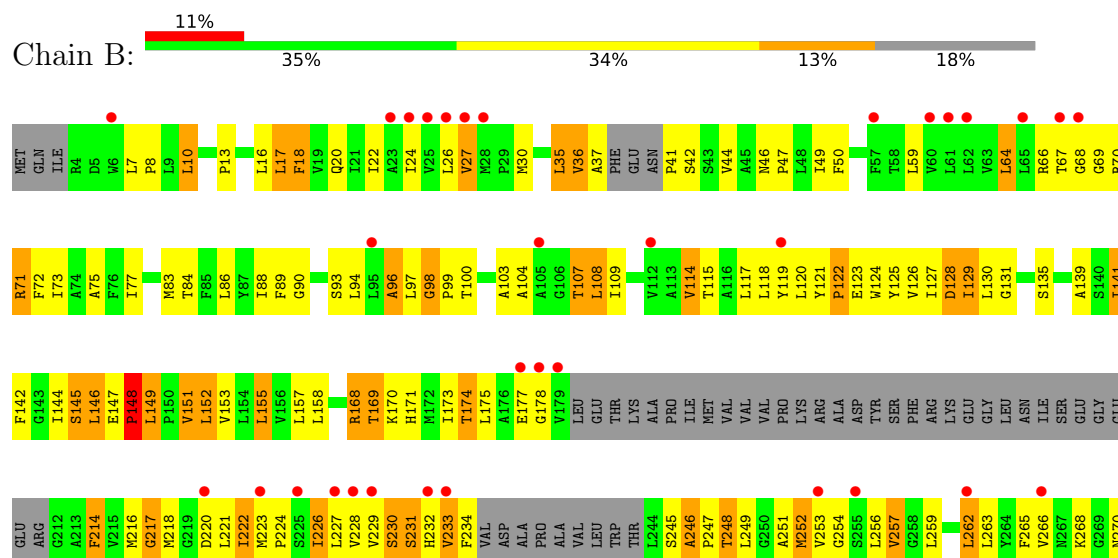
3 Residue-property plots [i](#)

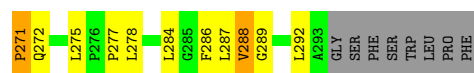
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

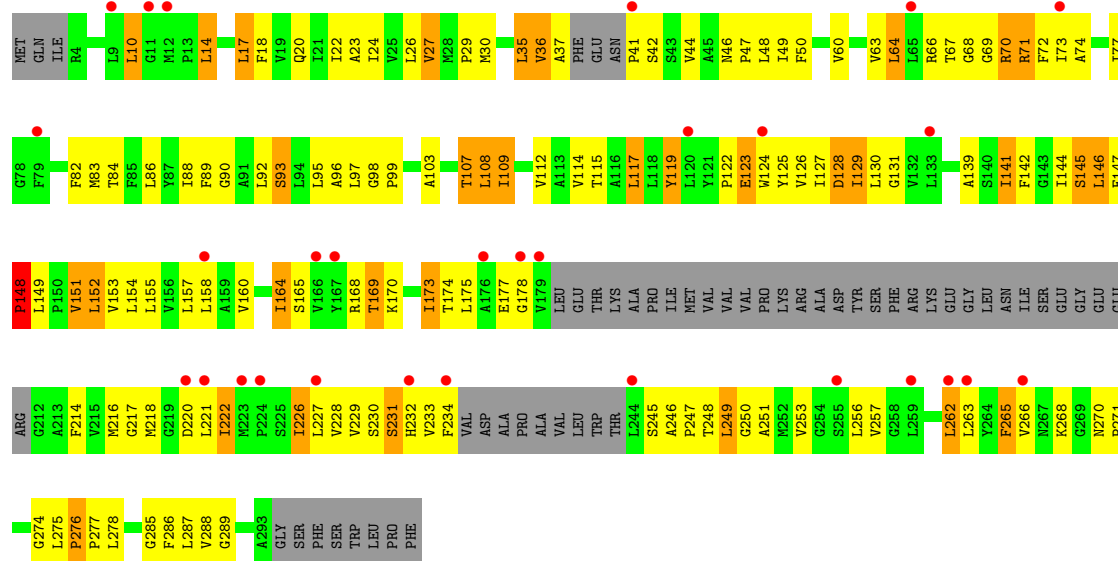


• Molecule 1: Putative uncharacterized protein

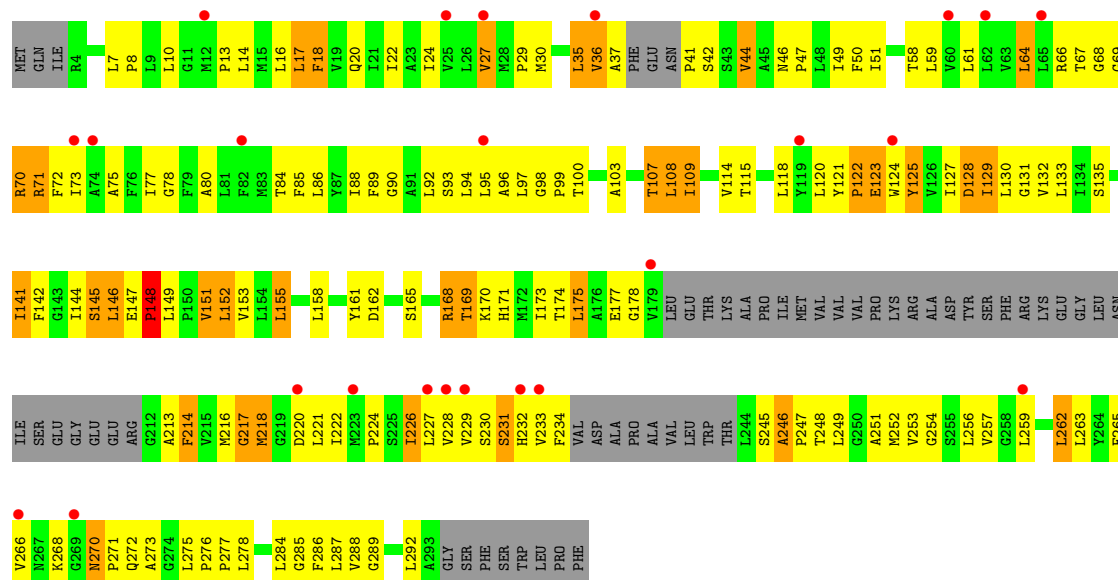




• Molecule 1: Putative uncharacterized protein

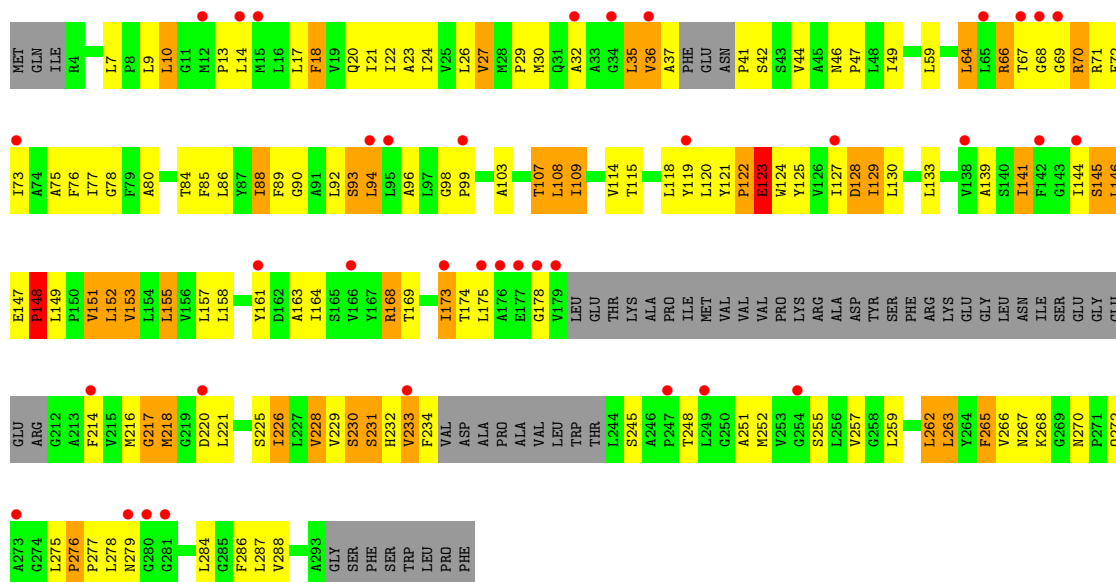


• Molecule 1: Putative uncharacterized protein

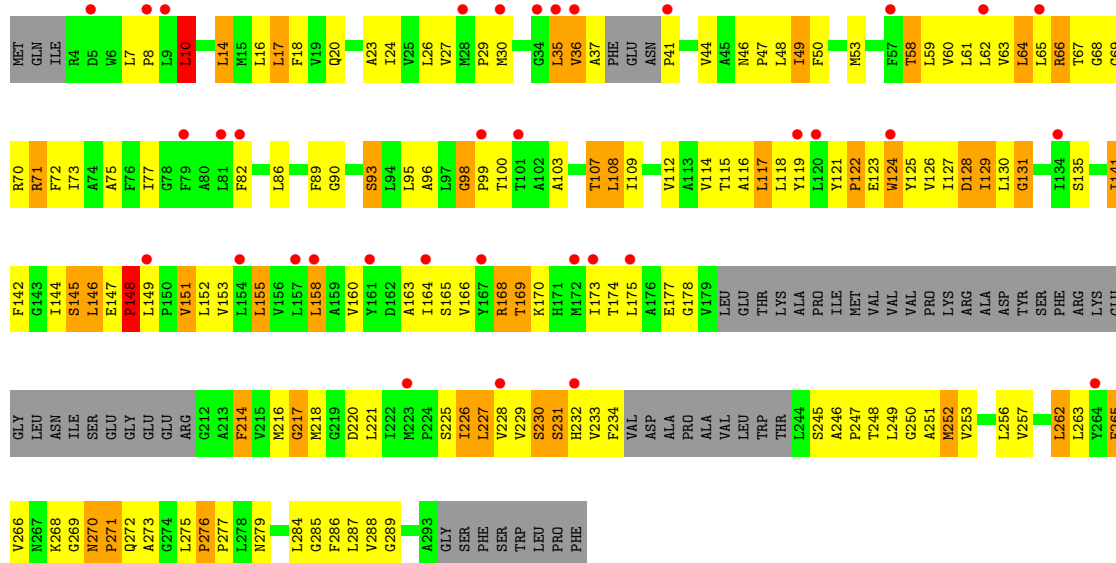


• Molecule 1: Putative uncharacterized protein

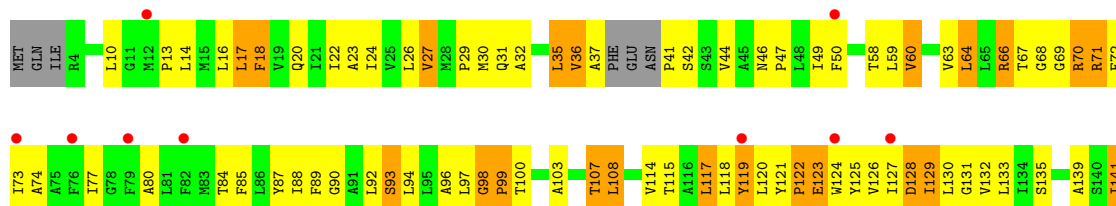


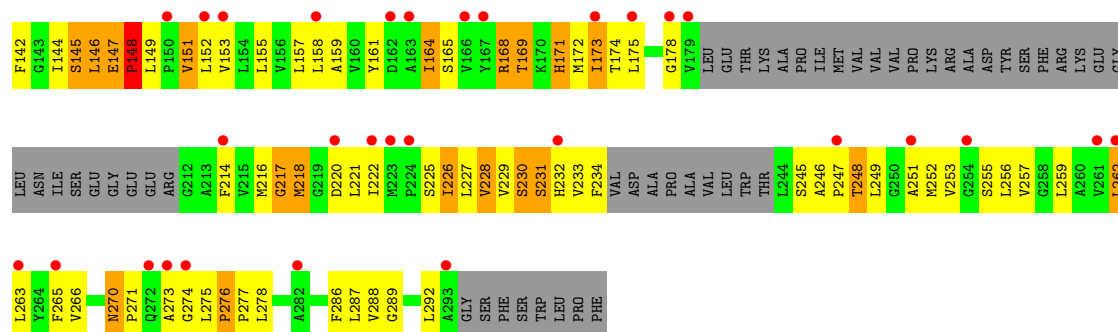


• Molecule 1: Putative uncharacterized protein

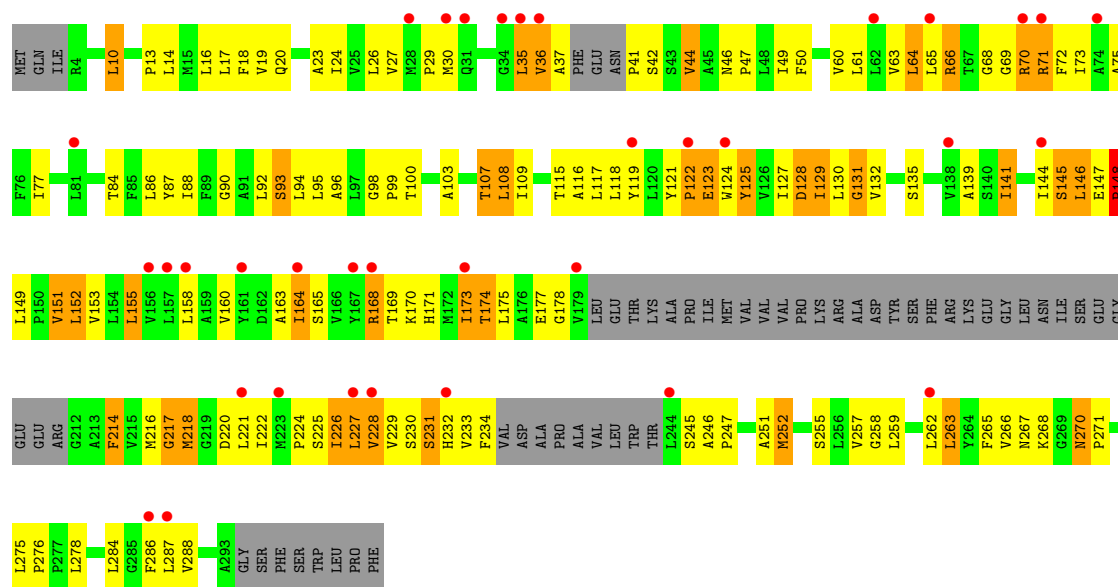


• Molecule 1: Putative uncharacterized protein





- Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	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) 78.7 (40.16-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.308 , 0.341 0.309 , 0.338	Depositor DCC
R_{free} test set	1341 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 94.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/1839	1.13	13/2511 (0.5%)
1	B	0.61	0/1839	1.12	16/2511 (0.6%)
1	C	0.61	0/1839	1.11	13/2511 (0.5%)
1	D	0.63	0/1839	1.11	12/2511 (0.5%)
1	E	0.63	0/1839	1.14	15/2511 (0.6%)
1	F	0.60	0/1839	1.13	13/2511 (0.5%)
1	G	0.61	0/1839	1.16	18/2511 (0.7%)
1	H	0.58	0/1839	1.06	9/2511 (0.4%)
All	All	0.61	0/14712	1.12	109/20088 (0.5%)

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 (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	LEU	N-CA-C	10.51	123.34	110.41
1	A	125	TYR	N-CA-C	-10.50	100.21	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	146	LEU	N-CA-C	10.22	122.99	110.41
1	F	270	ASN	CA-C-N	10.05	131.36	120.11
1	F	270	ASN	C-N-CA	10.05	131.36	120.11
1	C	125	TYR	N-CA-C	-10.00	100.83	113.23
1	E	146	LEU	N-CA-C	9.85	122.52	110.41
1	B	270	ASN	CA-C-N	9.81	131.09	120.11
1	B	270	ASN	C-N-CA	9.81	131.09	120.11
1	F	146	LEU	N-CA-C	9.78	122.44	110.41
1	A	146	LEU	N-CA-C	9.65	122.28	110.41
1	E	125	TYR	N-CA-C	-9.15	101.89	113.23
1	D	125	TYR	N-CA-C	-8.81	102.30	113.23
1	F	125	TYR	N-CA-C	-8.71	102.43	113.23
1	D	146	LEU	N-CA-C	8.54	120.91	110.41
1	H	146	LEU	N-CA-C	8.53	120.90	110.41
1	B	125	TYR	N-CA-C	-8.32	102.92	113.23
1	H	125	TYR	N-CA-C	-8.22	103.04	113.23
1	G	125	TYR	N-CA-C	-8.12	103.17	113.23
1	D	249	LEU	N-CA-C	-7.96	102.61	111.28
1	A	270	ASN	CA-C-N	7.82	128.87	120.11
1	A	270	ASN	C-N-CA	7.82	128.87	120.11
1	G	270	ASN	CA-C-N	7.66	128.69	120.11
1	G	270	ASN	C-N-CA	7.66	128.69	120.11
1	G	248	THR	N-CA-C	-7.03	103.81	112.88
1	D	248	THR	N-CA-C	-6.99	104.06	112.59
1	H	270	ASN	CA-C-N	6.84	127.77	120.11
1	H	270	ASN	C-N-CA	6.84	127.77	120.11
1	C	146	LEU	N-CA-C	6.84	118.82	110.41
1	B	248	THR	N-CA-C	-6.74	104.18	112.88
1	E	98	GLY	CA-C-N	6.73	128.25	119.84
1	E	98	GLY	C-N-CA	6.73	128.25	119.84
1	A	222	ILE	CB-CA-C	-6.50	103.69	111.81
1	C	276	PRO	N-CA-C	6.44	118.56	110.70
1	G	265	PHE	N-CA-C	6.30	117.82	111.07
1	A	276	PRO	N-CA-C	6.25	118.33	110.70
1	B	223	MET	CA-C-N	-6.25	113.52	120.45
1	B	223	MET	C-N-CA	-6.25	113.52	120.45
1	C	249	LEU	N-CA-C	-6.24	104.48	111.28
1	F	98	GLY	CA-C-N	6.21	127.60	119.84
1	F	98	GLY	C-N-CA	6.21	127.60	119.84
1	B	27	VAL	CB-CA-C	-6.20	104.03	111.97
1	D	175	LEU	N-CA-C	-6.10	105.67	113.23
1	B	249	LEU	N-CA-C	-6.09	104.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	ASN	CA-C-N	6.06	126.90	120.11
1	D	270	ASN	C-N-CA	6.06	126.90	120.11
1	D	27	VAL	CB-CA-C	-6.05	104.22	111.97
1	E	270	ASN	CA-C-N	6.03	126.86	120.11
1	E	270	ASN	C-N-CA	6.03	126.86	120.11
1	C	270	ASN	CA-C-N	6.03	127.37	119.84
1	C	270	ASN	C-N-CA	6.03	127.37	119.84
1	A	98	GLY	CA-C-N	5.99	127.32	119.84
1	A	98	GLY	C-N-CA	5.99	127.32	119.84
1	F	276	PRO	N-CA-C	5.88	117.87	110.70
1	E	276	PRO	N-CA-C	5.86	117.84	110.70
1	F	10	LEU	N-CA-C	-5.85	105.99	114.12
1	G	273	ALA	N-CA-C	5.85	117.52	111.03
1	D	131	GLY	N-CA-C	-5.83	105.73	112.73
1	G	249	LEU	N-CA-C	-5.83	104.92	111.28
1	G	98	GLY	CA-C-N	5.83	127.13	119.84
1	G	98	GLY	C-N-CA	5.83	127.13	119.84
1	F	131	GLY	N-CA-C	-5.82	105.74	112.73
1	H	160	VAL	N-CA-C	5.82	116.00	110.42
1	H	131	GLY	N-CA-C	-5.81	105.76	112.73
1	E	88	ILE	CB-CA-C	-5.79	104.57	111.81
1	C	164	ILE	N-CA-C	5.76	115.88	110.30
1	E	7	LEU	CA-C-N	-5.74	114.02	119.76
1	E	7	LEU	C-N-CA	-5.74	114.02	119.76
1	G	276	PRO	N-CA-C	5.70	117.66	110.70
1	E	27	VAL	CB-CA-C	-5.66	104.73	111.97
1	E	10	LEU	N-CA-C	-5.65	106.26	114.12
1	A	131	GLY	N-CA-C	-5.63	105.97	112.73
1	G	131	GLY	N-CA-C	-5.57	106.04	112.73
1	A	27	VAL	N-CA-C	-5.56	105.08	110.42
1	C	27	VAL	N-CA-C	-5.51	105.13	110.42
1	B	271	PRO	N-CA-C	5.51	119.21	111.33
1	D	51	ILE	N-CA-C	5.50	116.14	110.36
1	E	248	THR	N-CA-C	-5.50	105.88	112.59
1	B	222	ILE	CB-CA-C	-5.50	104.94	111.81
1	G	27	VAL	CB-CA-C	-5.47	104.96	111.97
1	H	10	LEU	N-CA-C	-5.46	106.53	114.12
1	G	164	ILE	N-CA-C	5.38	115.52	110.30
1	B	98	GLY	CA-C-N	5.36	126.54	119.84
1	B	98	GLY	C-N-CA	5.36	126.54	119.84
1	F	160	VAL	N-CA-C	5.29	116.02	110.62
1	G	71	ARG	N-CA-C	-5.29	106.77	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	GLY	N-CA-C	-5.24	106.44	112.73
1	C	98	GLY	CA-C-N	5.24	126.39	119.84
1	C	98	GLY	C-N-CA	5.24	126.39	119.84
1	D	27	VAL	N-CA-C	-5.24	105.39	110.42
1	C	131	GLY	N-CA-C	-5.23	106.45	112.73
1	D	213	ALA	N-CA-C	-5.20	106.44	112.89
1	F	248	THR	N-CA-C	-5.20	106.17	112.88
1	F	271	PRO	N-CA-C	5.17	118.73	111.33
1	A	249	LEU	N-CA-C	-5.15	105.66	111.28
1	C	160	VAL	N-CA-C	5.14	115.36	110.42
1	H	222	ILE	CB-CA-C	-5.14	105.38	111.81
1	B	114	VAL	N-CA-C	5.13	115.57	110.23
1	F	249	LEU	N-CA-C	-5.10	105.72	111.28
1	H	164	ILE	N-CA-C	5.08	115.29	110.42
1	E	265	PHE	N-CA-C	5.07	116.49	111.07
1	A	273	ALA	N-CA-C	5.07	116.66	111.03
1	G	60	VAL	N-CA-C	5.05	115.27	110.53
1	E	123	GLU	N-CA-C	-5.03	107.18	113.72
1	G	147	GLU	CA-C-N	5.03	126.12	119.84
1	G	147	GLU	C-N-CA	5.03	126.12	119.84
1	C	222	ILE	CB-CA-C	-5.02	105.53	111.81
1	B	123	GLU	N-CA-C	-5.01	107.20	113.72
1	A	114	VAL	N-CA-C	5.01	115.16	110.30

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 ⓘ

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	110	0
1	B	1802	0	1949	102	0
1	C	1802	0	1949	102	0
1	D	1802	0	1949	109	0
1	E	1802	0	1949	104	0
1	F	1802	0	1949	112	0
1	G	1802	0	1949	103	0
1	H	1802	0	1949	108	0
All	All	14416	0	15592	810	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 27.

All (810) 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
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:D:36:VAL:HG12	1:D:37:ALA:N	1.50	1.18
1:F:36:VAL:HG13	1:F:145:SER:CA	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CG1	1:H:37:ALA:H	1.58	1.12
1:H:36:VAL:HG12	1:H:37:ALA:N	1.55	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:B:36:VAL:HG12	1:B:37:ALA:N	1.54	1.08
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:F:36:VAL:HG12	1:F:37:ALA:N	1.58	1.05
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
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:B:36:VAL:HG13	1:B:145:SER:CB	1.98	0.92
1:E:36:VAL:HG22	1:E:144:ILE:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:41:PRO:C	1:B:146:LEU:HG	2.05	0.81
1:D:36:VAL:HG13	1:D:145:SER:CA	2.09	0.80
1:F:30:MET:HE1	1:F:141:ILE:HA	1.63	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:B:135:SER:HA	1:B:222:ILE:HD11	1.65	0.79
1:D:36:VAL:HG22	1:D:144:ILE:HG22	1.63	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:30:MET:HE1	1:B:141:ILE:HA	1.66	0.76
1:A:64:LEU:HD11	1:A:73:ILE:HG23	1.67	0.75
1:C:30:MET:HE1	1:C:141:ILE:HA	1.69	0.75
1:D:289:GLY:HA2	1:D:292:LEU:HD12	1.69	0.74
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:30:MET:HE1	1:H:141:ILE:HA	1.70	0.72
1:G:36:VAL:HG13	1:G:145:SER:CB	2.20	0.72
1:H:36:VAL:HG11	1:H:146:LEU:CD2	2.19	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:D:41:PRO:C	1:D:146:LEU:HG	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:36:VAL:HG22	1:C:144:ILE:C	2.15	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:D:42:SER:HA	1:D:146:LEU:HB3	1.71	0.70
1:F:20:GLN:HG2	1:F:225:SER:HB2	1.73	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:OD2	1:G:128:ASP:N	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:A:36:VAL:HG21	1:A:144:ILE:CG2	2.07	0.67
1:E:36:VAL:CG1	1:E:145:SER:HA	2.23	0.67
1:H:36:VAL:HG11	1:H:146:LEU:HD22	1.74	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: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:G:36:VAL:CG1	1:G:37:ALA:N	2.34	0.67
1:H:128:ASP:OD2	1:H:128:ASP:N	2.23	0.66
1:A:42:SER:HA	1:A:146:LEU:HB3	1.76	0.66
1:H:36:VAL:HG13	1:H:145:SER:HA	0.81	0.66
1:E:41:PRO:C	1:E:146:LEU:HG	2.21	0.66
1:B:42:SER:HA	1:B:146:LEU:HB3	1.76	0.66
1:D:36:VAL:CG2	1:D:144:ILE:HG22	2.25	0.66
1:H:20:GLN:O	1:H:24:ILE:HG12	1.96	0.66
1:F:129:ILE:HG22	1:F:130:LEU:HD23	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLY:HA2	1:H:107:THR:HG21	1.79	0.65
1:A:29:PRO:HB3	1:A:95:LEU:HB2	1.79	0.64
1:E:121:TYR:HA	1:E:124:TRP:CZ2	2.32	0.64
1:C:251:ALA:HB2	1:C:286:PHE:HB2	1.78	0.64
1:G:41:PRO:C	1:G:146:LEU:HG	2.23	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:A:41:PRO:C	1:A:146:LEU:HG	2.22	0.64
1:D:30:MET:HE1	1:D:141:ILE:HA	1.80	0.63
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:OD2	1:B:128:ASP:N	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:B:83:MET:HG2	1:C:48:LEU:HD23	1.81	0.62
1:D:97:LEU:HB2	1:D:103:ALA:HB2	1.80	0.62
1:E:121:TYR:HA	1:E:124:TRP:HZ2	1.65	0.62
1:D:128:ASP:OD2	1:D:128:ASP:N	2.31	0.62
1:G:120:LEU:HD21	1:H:164:ILE:HG12	1.82	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
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:A:168:ARG:HH12	1:D:70:ARG:NH2	1.98	0.61
1:G:36:VAL:CG2	1:G:144:ILE:HG22	2.29	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: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:64:LEU:HD21	1:C:73:ILE:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PRO:O	1:C:151:VAL:N	2.35	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:A:30:MET:HE1	1:A:141:ILE:HA	1.82	0.60
1:C:97:LEU:HB2	1:C:103:ALA:HB2	1.84	0.60
1:D:246:ALA:HB1	1:D:247:PRO:HD2	1.83	0.60
1:F:90:GLY:HA2	1:F:107:THR:HG21	1.83	0.60
1:G:29:PRO:O	1:G:32:ALA:HB3	2.00	0.60
1:G:31:GLN:HG3	1:G:144:ILE:HD13	1.83	0.60
1:B:71:ARG:O	1:B:75:ALA:N	2.34	0.60
1:C:72:PHE:CZ	1:D:59:LEU:HD23	2.36	0.60
1:C:47:PRO:O	1:C:50:PHE:HB3	2.01	0.60
1:E:24:ILE:HD13	1:E:229:VAL:HG22	1.84	0.60
1:E:129:ILE:HG22	1:E:130:LEU:HD23	1.84	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:30:MET:HE1	1:G:141:ILE:HA	1.83	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:D:165:SER:O	1:D:169:THR:HG23	2.02	0.59
1:E:36:VAL:HG13	1:E:145:SER:CB	2.32	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
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:B:265:PHE:O	1:B:268:LYS:HG2	2.03	0.58
1:D:217:GLY:O	1:D:220:ASP:N	2.37	0.58
1:E:86:LEU:HD21	1:E:108:LEU:HA	1.86	0.57
1:B:86:LEU:HD21	1:B:108:LEU:HA	1.84	0.57
1:H:61:LEU:O	1:H:64:LEU:HB3	2.03	0.57
1:C:229:VAL:O	1:C:231:SER:N	2.37	0.57
1:E:24:ILE:HA	1:E:27:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ALA:O	1:C:119:TYR:OH	2.21	0.57
1:D:275:LEU:O	1:D:278:LEU:N	2.38	0.57
1:F:253:VAL:HA	1:F:256:LEU:HD12	1.86	0.57
1:H:36:VAL:CG1	1:H:146:LEU:CD2	2.82	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:B:148:PRO:O	1:B:151:VAL:N	2.38	0.57
1:G:251:ALA:HB2	1:G:286:PHE:HB2	1.86	0.57
1:G:13:PRO:HB3	1:G:259:LEU:HD22	1.87	0.57
1:C:23:ALA:O	1:C:27:VAL:HG23	2.04	0.57
1:H:68:GLY:HA3	1:H:73:ILE:HD11	1.86	0.57
1:F:147:GLU:HB3	1:F:148:PRO:HD2	1.86	0.56
1:G:229:VAL:O	1:G:231:SER:N	2.36	0.56
1:A:228:VAL:HG21	1:A:252:MET:HG3	1.87	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:H:19:VAL:HG22	1:H:132:VAL:HA	1.88	0.56
1:A:247:PRO:O	1:A:289:GLY:HA3	2.04	0.56
1:B:170:LYS:HZ1	1:B:271:PRO:HG2	1.71	0.56
1:B:262:LEU:HD23	1:B:277:PRO:HG2	1.88	0.56
1:C:93:SER:HB3	1:C:107:THR:HG22	1.88	0.56
1:D:129:ILE:HG22	1:D:130:LEU:HD23	1.87	0.56
1:H:24:ILE:HA	1:H:27:VAL:HG23	1.86	0.56
1:E:20:GLN:O	1:E:24:ILE:HG12	2.06	0.56
1:F:36:VAL:HG11	1:F:146:LEU:CD2	2.35	0.56
1:A:148:PRO:O	1:A:151:VAL:N	2.39	0.56
1:D:148:PRO:O	1:D:151:VAL:N	2.38	0.56
1:G:36:VAL:HG13	1:G:145:SER:OG	2.06	0.56
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:B:84:THR:O	1:B:88:ILE:HG12	2.05	0.56
1:G:70:ARG:NH2	1:H:168:ARG:HH12	2.03	0.56
1:H:42:SER:HB2	1:H:147:GLU:HG2	1.87	0.56
1:G:20:GLN:CD	1:G:252:MET:HG2	2.32	0.55
1:H:124:TRP:HA	1:H:127:ILE:HG12	1.87	0.55
1:D:20:GLN:CD	1:D:252:MET:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LEU:HD11	1:E:73:ILE:HG23	1.88	0.55
1:G:35:LEU:O	1:G:36:VAL:HB	2.07	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:G:124:TRP:HA	1:G:127:ILE:HG12	1.88	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:C:41:PRO:C	1:C:146:LEU:HG	2.32	0.55
1:F:251:ALA:HB2	1:F:286:PHE:HB2	1.88	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:D:254:GLY:HA3	1:D:285:GLY:HA3	1.89	0.54
1:E:66:ARG:HH22	1:F:66:ARG:HD3	1.72	0.54
1:E:72:PHE:HZ	1:F:59:LEU:HB2	1.71	0.54
1:E:90:GLY:HA2	1:E:107:THR:HG21	1.89	0.54
1:E:225:SER:HA	1:E:228:VAL:HB	1.89	0.54
1:F:170:LYS:NZ	1:F:271:PRO:HG2	2.23	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:H:41:PRO:C	1:H:146:LEU:HG	2.32	0.54
1:E:20:GLN:CD	1:E:252:MET:HG2	2.33	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: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
1:F:61:LEU:O	1:F:64:LEU:HB3	2.07	0.54
1:G:117:LEU:HD11	1:G:126:VAL:HG11	1.89	0.54
1:H:147:GLU:HB3	1:H:148:PRO:HD2	1.89	0.54
1:D:29:PRO:HB3	1:D:95:LEU:HD22	1.90	0.54
1:E:70:ARG:HH21	1:F:168:ARG:HH22	1.55	0.54
1:E:251:ALA:HB2	1:E:286:PHE:HB2	1.89	0.54
1:F:16:LEU:HA	1:F:221:LEU:HD11	1.89	0.54
1:C:83:MET:O	1:C:86:LEU:HB2	2.08	0.54
1:H:86:LEU:CD2	1:H:108:LEU:HA	2.38	0.54
1:E:42:SER:HA	1:E:146:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:VAL:CG1	1:F:37:ALA:N	2.35	0.54
1:B:251:ALA:HB2	1:B:286:PHE:HB2	1.89	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:D:265:PHE:O	1:D:268:LYS:HG2	2.09	0.53
1:A:123:GLU:HB2	1:A:126:VAL:HG23	1.91	0.53
1:E:64:LEU:HD21	1:E:73:ILE:HA	1.90	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:A:24:ILE:HA	1:A:27:VAL:HG23	1.89	0.53
1:A:90:GLY:HA2	1:A:107:THR:HG21	1.91	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:B:289:GLY:CA	1:B:292:LEU:HD12	2.27	0.53
1:G:94:LEU:HD22	1:G:99:PRO:HA	1.89	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:B:90:GLY:HA2	1:B:107:THR:HG21	1.91	0.52
1:D:68:GLY:HA3	1:D:73:ILE:HD11	1.92	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:B:275:LEU:O	1:B:278:LEU:N	2.42	0.52
1:D:121:TYR:HD1	1:D:124:TRP:HZ2	1.58	0.52
1:A:18:PHE:O	1:A:22:ILE:HG12	2.10	0.52
1:H:127:ILE:HG22	1:H:214:PHE:HE2	1.75	0.52
1:A:89:PHE:HD1	1:A:92:LEU:HD12	1.75	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:H:36:VAL:CG1	1:H:37:ALA:N	2.31	0.52
1:H:60:VAL:O	1:H:63:VAL:HG12	2.10	0.52
1:B:16:LEU:HA	1:B:221:LEU:HD11	1.92	0.52
1:C:42:SER:HA	1:C:146:LEU:HB3	1.91	0.52
1:C:142:PHE:HA	1:C:145:SER:HB3	1.90	0.52
1:F:36:VAL:HG22	1:F:144:ILE:C	2.35	0.52
1:F:118:LEU:HD12	1:F:130:LEU:HD12	1.92	0.52
1:D:265:PHE:HB3	1:D:272:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ALA:O	1:G:84:THR:HG23	2.10	0.52
1:H:42:SER:HA	1:H:146:LEU:HB3	1.91	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:E:265:PHE:HB3	1:E:272:GLN:OE1	2.09	0.51
1:F:23:ALA:O	1:F:27:VAL:HG23	2.10	0.51
1:A:93:SER:OG	1:A:103:ALA:HB1	2.11	0.51
1:C:36:VAL:CG1	1:C:37:ALA:N	2.30	0.51
1:G:246:ALA:C	1:G:248:THR:H	2.19	0.51
1:H:118:LEU:HD12	1:H:130:LEU:HD12	1.92	0.51
1:A:127:ILE:HG22	1:A:214:PHE:HE2	1.75	0.51
1:E:44:VAL:O	1:E:47:PRO:HD2	2.09	0.51
1:H:36:VAL:HG13	1:H:145:SER:CB	2.40	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:C:123:GLU:HB2	1:C:126:VAL:HG23	1.93	0.51
1:H:36:VAL:HG23	1:H:144:ILE:HG22	1.81	0.51
1:H:218:MET:HA	1:H:221:LEU:HB3	1.93	0.51
1:A:168:ARG:HH12	1:D:70:ARG:HH22	1.58	0.51
1:B:68:GLY:HA3	1:B:73:ILE:HD11	1.92	0.51
1:D:98:GLY:O	1:D:100:THR:N	2.43	0.51
1:G:17:LEU:HD21	1:G:256:LEU:HD11	1.93	0.51
1:G:26:LEU:C	1:G:29:PRO:HD2	2.36	0.51
1:C:84:THR:O	1:C:88:ILE:HG12	2.10	0.51
1:E:26:LEU:C	1:E:29:PRO:HD2	2.36	0.51
1:E:93:SER:HB3	1:E:107:THR:HG22	1.93	0.51
1:F:247:PRO:O	1:F:289:GLY:HA3	2.11	0.51
1:B:7:LEU:HB2	1:B:8:PRO:HD3	1.93	0.50
1:E:217:GLY:O	1:E:220:ASP:N	2.43	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: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:F:165:SER:O	1:F:169:THR:HG23	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:PHE:HZ	1:F:114:VAL:HG21	1.76	0.50
1:F:268:LYS:HG3	1:F:269:GLY:O	2.12	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:98:GLY:O	1:H:100:THR:N	2.44	0.50
1:H:217:GLY:O	1:H:220:ASP:N	2.45	0.50
1:A:44:VAL:O	1:A:47:PRO:HD2	2.12	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:D:7:LEU:HB2	1:D:8:PRO:HD3	1.94	0.50
1:C:26:LEU:C	1:C:29:PRO:HD2	2.37	0.49
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:E:220:ASP:OD2	1:E:221:LEU:N	2.45	0.49
1:E:265:PHE:O	1:E:268:LYS:HG2	2.11	0.49
1:F:35:LEU:O	1:F:36:VAL:HB	2.12	0.49
1:H:229:VAL:O	1:H:231:SER:N	2.45	0.49
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.93	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:121:TYR:HD1	1:A:124:TRP:HZ2	1.59	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:E:220:ASP:OD2	1:E:220:ASP:C	2.56	0.49
1:G:41:PRO:N	1:G:146:LEU:HG	2.26	0.49
1:B:117:LEU:CD1	1:B:126:VAL:HG11	2.43	0.49
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.94	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:268:LYS:HE2	1:B:272:GLN:HE22	1.77	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:D:220:ASP:OD2	1:D:220:ASP:C	2.56	0.49
1:H:170:LYS:HZ1	1:H:271:PRO:HG2	1.78	0.49
1:B:155:LEU:HD11	1:B:224:PRO:HA	1.95	0.49
1:G:24:ILE:HA	1:G:27:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:230:SER:HA	1:B:233:VAL:HG12	1.94	0.48
1:C:36:VAL:CG1	1:C:146:LEU:HD22	2.43	0.48
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.95	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: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:44:VAL:C	1:A:47:PRO:HD2	2.39	0.48
1:A:93:SER:HB3	1:A:107:THR:HG22	1.95	0.48
1:B:220:ASP:C	1:B:220:ASP:OD2	2.55	0.48
1:C:14:LEU:O	1:C:18:PHE:HB2	2.14	0.48
1:F:246:ALA:HB1	1:F:247:PRO:HD2	1.95	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:F:86:LEU:CD2	1:F:108:LEU:HA	2.44	0.48
1:G:142:PHE:HB2	1:G:226:ILE:HD11	1.96	0.48
1:G:159:ALA:HB1	1:G:276:PRO:HG3	1.95	0.48
1:G:275:LEU:HB2	1:G:276:PRO:HD3	1.96	0.48
1:C:142:PHE:HB2	1:C:226:ILE:CD1	2.44	0.47
1:B:47:PRO:O	1:B:50:PHE:HB3	2.14	0.47
1:C:165:SER:O	1:C:169:THR:HG23	2.13	0.47
1:G:18:PHE:O	1:G:22:ILE:HG12	2.14	0.47
1:C:275:LEU:HB2	1:C:276:PRO:HD3	1.95	0.47
1:E:121:TYR:C	1:E:124:TRP:HE1	2.22	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:B:152:LEU:HD22	1:B:152:LEU:HA	1.77	0.47
1:D:24:ILE:O	1:D:27:VAL:N	2.46	0.47
1:D:35:LEU:O	1:D:36:VAL:HB	2.13	0.47
1:H:228:VAL:HG21	1:H:252:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LYS:HZ2	1:D:271:PRO:HG2	1.78	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:89:PHE:CZ	1:F:114:VAL:HG21	2.49	0.47
1:F:151:VAL:HG12	1:F:227:LEU:HD12	1.96	0.47
1:D:18:PHE:O	1:D:22:ILE:HG12	2.15	0.47
1:E:68:GLY:HA3	1:E:73:ILE:HD11	1.97	0.47
1:H:151:VAL:HG12	1:H:227:LEU:HD12	1.97	0.47
1:A:139:ALA:HA	1:A:226:ILE:HD12	1.96	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:B:10:LEU:HD23	1:B:10:LEU:HA	1.83	0.47
1:C:265:PHE:O	1:C:268:LYS:HG2	2.15	0.47
1:F:68:GLY:HA2	1:F:69:GLY:HA3	1.57	0.47
1:H:284:LEU:HD23	1:H:284:LEU:HA	1.71	0.47
1:A:161:TYR:OH	1:D:71:ARG:NH1	2.48	0.46
1:C:89:PHE:C	1:C:107:THR:HB	2.40	0.46
1:F:24:ILE:HA	1:F:27:VAL:HG23	1.98	0.46
1:F:72:PHE:CZ	1:G:59:LEU:HD23	2.50	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:E:66:ARG:HH22	1:F:66:ARG:CD	2.27	0.46
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.70	0.46
1:G:142:PHE:HB2	1:G:226:ILE:CD1	2.45	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:C:246:ALA:C	1:C:248:THR:H	2.22	0.46
1:F:41:PRO:N	1:F:146:LEU:HG	2.31	0.46
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.97	0.46
1:C:89:PHE:CD1	1:C:92:LEU:HD12	2.51	0.46
1:D:89:PHE:HZ	1:D:114:VAL:HG21	1.80	0.46
1:E:30:MET:HE1	1:E:141:ILE:HA	1.98	0.46
1:F:142:PHE:HB2	1:F:226:ILE:CD1	2.46	0.46
1:H:26:LEU:C	1:H:29:PRO:HD2	2.40	0.46
1:A:84:THR:O	1:A:88:ILE:HG12	2.15	0.46
1:B:127:ILE:HG22	1:B:214:PHE:HE2	1.81	0.46
1:E:275:LEU:HB2	1:E:276:PRO:HD3	1.97	0.46
1:F:250:GLY:O	1:F:285:GLY:HA3	2.15	0.46
1:F:284:LEU:HD23	1:F:284:LEU:HA	1.68	0.46
1:G:220:ASP:C	1:G:220:ASP:OD2	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:HB2	1:A:146:LEU:HD12	1.98	0.46
1:C:68:GLY:HA2	1:C:69:GLY:HA3	1.63	0.46
1:H:47:PRO:O	1:H:50:PHE:HB3	2.16	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:C:20:GLN:O	1:C:24:ILE:HG12	2.16	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:G:66:ARG:HH22	1:H:66:ARG:CD	2.29	0.46
1:H:84:THR:O	1:H:88:ILE:HG12	2.16	0.46
1:H:121:TYR:HA	1:H:124:TRP:HZ2	1.81	0.46
1:A:82:PHE:CZ	1:B:157:LEU:HD11	2.51	0.45
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:F:41:PRO:C	1:F:146:LEU:HG	2.41	0.45
1:A:121:TYR:HA	1:A:124:TRP:CZ2	2.50	0.45
1:C:72:PHE:HZ	1:D:59:LEU:HD23	1.79	0.45
1:C:82:PHE:HE1	1:C:112:VAL:HA	1.80	0.45
1:C:218:MET:HA	1:C:221:LEU:HB3	1.98	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:B:124:TRP:HA	1:B:127:ILE:HG12	1.98	0.45
1:E:85:PHE:HE1	1:E:133:LEU:HD23	1.82	0.45
1:F:10:LEU:O	1:F:14:LEU:HB2	2.16	0.45
1:F:49:ILE:O	1:F:53:MET:HG2	2.16	0.45
1:F:217:GLY:O	1:F:220:ASP:N	2.49	0.45
1:A:15:MET:O	1:A:19:VAL:HG23	2.17	0.45
1:B:122:PRO:HD2	1:B:124:TRP:CE2	2.52	0.45
1:C:36:VAL:HG13	1:C:145:SER:HA	0.71	0.45
1:C:89:PHE:HZ	1:C:114:VAL:HG21	1.81	0.45
1:D:121:TYR:HA	1:D:124:TRP:HZ2	1.80	0.45
1:D:122:PRO:HB2	1:D:123:GLU:H	1.57	0.45
1:E:122:PRO:HD2	1:E:124:TRP:CZ2	2.51	0.45
1:D:155:LEU:HD11	1:D:224:PRO:HA	1.98	0.45
1:E:75:ALA:O	1:E:78:GLY:N	2.50	0.45
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.84	0.45
1:G:122:PRO:HB2	1:G:123:GLU:H	1.60	0.45
1:C:36:VAL:HG11	1:C:146:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:121:TYR:HA	1:A:122:PRO:HD2	1.82	0.45
1:C:42:SER:OG	1:C:147:GLU:HB2	2.17	0.45
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.99	0.45
1:D:20:GLN:NE2	1:D:252:MET:HG2	2.32	0.45
1:F:64:LEU:HD13	1:F:65:LEU:N	2.32	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:68:GLY:HA2	1:H:69:GLY:HA3	1.60	0.45
1:A:121:TYR:HA	1:A:124:TRP:HZ2	1.82	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:E:86:LEU:HD12	1:F:48:LEU:HD21	1.98	0.44
1:H:30:MET:HB3	1:H:35:LEU:HD22	1.99	0.44
1:A:64:LEU:HD23	1:A:72:PHE:CE2	2.52	0.44
1:A:89:PHE:HZ	1:A:114:VAL:HG21	1.82	0.44
1:D:36:VAL:CG1	1:D:146:LEU:CD2	2.94	0.44
1:D:127:ILE:HG22	1:D:214:PHE:HE2	1.82	0.44
1:E:13:PRO:HB3	1:E:259:LEU:HD22	1.99	0.44
1:H:13:PRO:HD3	1:H:259:LEU:HD21	1.98	0.44
1:H:23:ALA:O	1:H:27:VAL:HG23	2.17	0.44
1:H:86:LEU:HD23	1:H:86:LEU:HA	1.79	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:F:26:LEU:C	1:F:29:PRO:HD2	2.42	0.44
1:H:35:LEU:O	1:H:36:VAL:HB	2.17	0.44
1:A:61:LEU:O	1:A:64:LEU:HB3	2.17	0.44
1:D:16:LEU:HD23	1:D:256:LEU:HD23	1.98	0.44
1:D:68:GLY:HA2	1:D:69:GLY:HA3	1.73	0.44
1:E:44:VAL:C	1:E:47:PRO:HD2	2.42	0.44
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.76	0.44
1:B:98:GLY:O	1:B:100:THR:N	2.50	0.44
1:C:107:THR:OG1	1:C:108:LEU:N	2.50	0.44
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:220:ASP:OD2	1:B:221:LEU:N	2.50	0.44
1:C:173:ILE:HD12	1:C:173:ILE:HA	1.82	0.44
1:C:218:MET:O	1:C:222:ILE:HG13	2.16	0.44
1:F:24:ILE:O	1:F:27:VAL:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:PRO:HD3	1:G:230:SER:O	2.18	0.44
1:G:173:ILE:HD12	1:G:173:ILE:HA	1.67	0.44
1:H:152:LEU:HD22	1:H:152:LEU:HA	1.80	0.44
1:C:60:VAL:HA	1:C:63:VAL:HG12	1.99	0.44
1:G:262:LEU:HD23	1:G:277:PRO:HG2	2.00	0.44
1:A:220:ASP:OD2	1:A:220:ASP:C	2.59	0.44
1:D:170:LYS:HZ1	1:D:271:PRO:C	2.26	0.44
1:E:41:PRO:N	1:E:146:LEU:HG	2.33	0.44
1:E:139:ALA:HA	1:E:226:ILE:HD12	2.00	0.44
1:G:69:GLY:CA	1:G:72:PHE:HB3	2.48	0.44
1:G:225:SER:HA	1:G:228:VAL:HB	1.99	0.44
1:H:220:ASP:OD2	1:H:221:LEU:N	2.51	0.44
1:A:275:LEU:O	1:A:278:LEU:N	2.51	0.44
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.78	0.44
1:F:270:ASN:HA	1:F:271:PRO:HD2	1.78	0.44
1:G:16:LEU:HA	1:G:221:LEU:HD11	1.98	0.44
1:H:155:LEU:HD11	1:H:224:PRO:HA	1.99	0.44
1:A:173:ILE:HD12	1:A:173:ILE:HA	1.80	0.43
1:B:17:LEU:HD23	1:B:17:LEU:HA	1.71	0.43
1:C:152:LEU:HD22	1:C:152:LEU:HA	1.89	0.43
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.87	0.43
1:F:166:VAL:HG21	1:F:273:ALA:HA	2.00	0.43
1:G:85:PHE:HE1	1:G:133:LEU:HD23	1.82	0.43
1:H:124:TRP:CE3	1:H:127:ILE:HG13	2.53	0.43
1:A:14:LEU:O	1:A:18:PHE:HB2	2.18	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: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:47:PRO:O	1:F:50:PHE:HB3	2.19	0.43
1:F:122:PRO:HD2	1:F:124:TRP:CE2	2.53	0.43
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:A:151:VAL:HG12	1:A:227:LEU:HD12	2.01	0.43
1:E:109:ILE:HD13	1:E:109:ILE:HA	1.71	0.43
1:G:24:ILE:O	1:G:27:VAL:HB	2.18	0.43
1:G:289:GLY:HA2	1:G:292:LEU:HD12	2.00	0.43
1:H:42:SER:OG	1:H:147:GLU:HB2	2.17	0.43
1:H:171:HIS:HA	1:H:174:THR:HG23	2.00	0.43
1:H:220:ASP:OD2	1:H:220:ASP:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HD21	1:B:104:ALA:HB2	2.00	0.43
1:C:10:LEU:HD23	1:C:10:LEU:HA	1.81	0.43
1:C:17:LEU:CD2	1:C:256:LEU:HD11	2.45	0.43
1:D:58:THR:O	1:D:61:LEU:N	2.51	0.43
1:E:93:SER:OG	1:E:103:ALA:HB1	2.18	0.43
1:G:36:VAL:CG1	1:G:145:SER:OG	2.65	0.43
1:H:139:ALA:HA	1:H:226:ILE:HD12	2.00	0.43
1:A:26:LEU:C	1:A:29:PRO:HD2	2.43	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:B:89:PHE:CZ	1:B:114:VAL:HG21	2.53	0.43
1:C:247:PRO:HB2	1:C:289:GLY:HA3	2.01	0.43
1:E:18:PHE:O	1:E:22:ILE:HG12	2.19	0.43
1:G:36:VAL:HA	1:G:145:SER:HB2	2.00	0.43
1:A:89:PHE:CD1	1:A:92:LEU:HD12	2.54	0.43
1:A:250:GLY:O	1:A:285:GLY:HA3	2.18	0.43
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.73	0.43
1:C:170:LYS:NZ	1:C:271:PRO:HG2	2.32	0.43
1:D:109:ILE:HD13	1:D:109:ILE:HA	1.79	0.43
1:E:218:MET:HA	1:E:221:LEU:HB3	2.00	0.43
1:F:127:ILE:HG22	1:F:214:PHE:HE2	1.84	0.43
1:F:265:PHE:HB3	1:F:272:GLN:OE1	2.19	0.43
1:A:124:TRP:CE3	1:A:127:ILE:HG13	2.54	0.43
1:D:152:LEU:HD22	1:D:152:LEU:HA	1.85	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:A:7:LEU:HB2	1:A:8:PRO:HD3	2.01	0.43
1:B:171:HIS:O	1:B:174:THR:HG23	2.19	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:H:275:LEU:HA	1:H:275:LEU:HD23	1.78	0.43
1:B:107:THR:OG1	1:B:108:LEU:N	2.51	0.42
1:C:220:ASP:OD2	1:C:220:ASP:C	2.61	0.42
1:D:44:VAL:O	1:D:47:PRO:HD2	2.18	0.42
1:G:262:LEU:HD21	1:G:274:GLY:HA2	2.00	0.42
1:H:165:SER:O	1:H:169:THR:HG23	2.19	0.42
1:A:259:LEU:HB2	1:A:278:LEU:HD11	2.01	0.42
1:B:246:ALA:C	1:B:248:THR:H	2.25	0.42
1:C:250:GLY:O	1:C:285:GLY:HA3	2.19	0.42
1:D:80:ALA:O	1:D:84:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ASP:OD2	1:D:273:ALA:HB1	2.19	0.42
1:D:220:ASP:OD2	1:D:221:LEU:N	2.52	0.42
1:A:214:PHE:HD1	1:A:214:PHE:HA	1.66	0.42
1:B:20:GLN:CD	1:B:252:MET:HG2	2.44	0.42
1:D:47:PRO:O	1:D:50:PHE:HB3	2.20	0.42
1:E:80:ALA:O	1:E:84:THR:HG23	2.18	0.42
1:G:64:LEU:HD21	1:G:73:ILE:HA	2.01	0.42
1:A:23:ALA:O	1:A:27:VAL:HG23	2.19	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:D:247:PRO:O	1:D:289:GLY:HA3	2.19	0.42
1:E:68:GLY:HA2	1:E:69:GLY:HA3	1.69	0.42
1:A:60:VAL:HA	1:A:63:VAL:HG12	2.01	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:98:GLY:O	1:A:100:THR:N	2.53	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:B:254:GLY:O	1:B:257:VAL:HG12	2.20	0.42
1:D:275:LEU:HB2	1:D:276:PRO:HD3	2.00	0.42
1:G:87:TYR:N	1:G:87:TYR:CD2	2.88	0.42
1:H:24:ILE:O	1:H:27:VAL:N	2.51	0.42
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.75	0.42
1:B:218:MET:HA	1:B:221:LEU:HB3	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:G:151:VAL:HG12	1:G:227:LEU:HD12	2.01	0.42
1:A:15:MET:SD	1:A:128:ASP:HB3	2.60	0.42
1:B:121:TYR:HA	1:B:124:TRP:CZ2	2.54	0.42
1:D:36:VAL:HG13	1:D:145:SER:OG	2.19	0.42
1:D:259:LEU:HA	1:D:278:LEU:HD21	2.02	0.42
1:F:20:GLN:CD	1:F:252:MET:HG2	2.45	0.42
1:F:163:ALA:HB2	1:F:276:PRO:HG2	2.01	0.42
1:H:98:GLY:C	1:H:100:THR:H	2.28	0.42
1:H:270:ASN:HA	1:H:271:PRO:HD2	1.84	0.42
1:C:44:VAL:C	1:C:47:PRO:HD2	2.44	0.42
1:E:23:ALA:O	1:E:27:VAL:HG23	2.20	0.42
1:E:75:ALA:O	1:E:76:PHE:C	2.62	0.42
1:E:155:LEU:HD22	1:E:279:ASN:ND2	2.35	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:A:36:VAL:HG22	1:A:144:ILE:C	2.45	0.41
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.85	0.41
1:D:85:PHE:HE1	1:D:133:LEU:HD23	1.85	0.41
1:D:122:PRO:HD2	1:D:124:TRP:CE2	2.55	0.41
1:E:21:ILE:HG22	1:E:22:ILE:HD13	2.02	0.41
1:F:71:ARG:NH1	1:G:161:TYR:OH	2.52	0.41
1:F:220:ASP:HB2	1:F:275:LEU:HD21	2.02	0.41
1:A:220:ASP:OD2	1:A:221:LEU:N	2.53	0.41
1:C:109:ILE:HA	1:C:109:ILE:HD13	1.77	0.41
1:C:129:ILE:HD13	1:C:129:ILE:HA	1.80	0.41
1:C:142:PHE:HB2	1:C:226:ILE:HG12	2.03	0.41
1:D:284:LEU:HA	1:D:284:LEU:HD23	1.75	0.41
1:E:122:PRO:HB2	1:E:123:GLU:H	1.62	0.41
1:F:58:THR:O	1:F:62:LEU:HG	2.19	0.41
1:F:155:LEU:HD22	1:F:279:ASN:ND2	2.36	0.41
1:G:44:VAL:O	1:G:47:PRO:HD2	2.20	0.41
1:G:168:ARG:HB3	1:G:168:ARG:CZ	2.50	0.41
1:H:258:GLY:HA3	1:H:278:LEU:HA	2.02	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:B:68:GLY:HA2	1:B:69:GLY:HA3	1.76	0.41
1:B:148:PRO:O	1:B:149:LEU:C	2.63	0.41
1:C:142:PHE:HB2	1:C:226:ILE:HD11	2.03	0.41
1:C:157:LEU:HD12	1:C:157:LEU:HA	1.81	0.41
1:E:139:ALA:O	1:E:226:ILE:HG13	2.21	0.41
1:E:217:GLY:O	1:E:218:MET:C	2.64	0.41
1:H:87:TYR:N	1:H:87:TYR:CD2	2.88	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:220:ASP:OD2	1:F:220:ASP:C	2.63	0.41
1:F:229:VAL:O	1:F:231:SER:N	2.52	0.41
1:A:118:LEU:HD12	1:A:130:LEU:HD12	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:E:259:LEU:HB2	1:E:278:LEU:HD11	2.03	0.41
1:F:27:VAL:O	1:F:144:ILE:HD11	2.21	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
1:H:36:VAL:HG22	1:H:144:ILE:C	2.45	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: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:D:107:THR:OG1	1:D:108:LEU:N	2.54	0.41
1:G:68:GLY:HA3	1:G:73:ILE:HD11	2.02	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:E:152:LEU:HD22	1:E:152:LEU:HA	1.91	0.41
1:G:93:SER:OG	1:G:103:ALA:HB1	2.21	0.41
1:H:64:LEU:HD13	1:H:65:LEU:N	2.36	0.41
1:H:92:LEU:HD23	1:H:92:LEU:HA	1.90	0.41
1:H:263:LEU:O	1:H:267:ASN:ND2	2.48	0.41
1:A:80:ALA:O	1:A:84:THR:HG23	2.21	0.41
1:F:17:LEU:HD23	1:F:17:LEU:HA	1.76	0.41
1:G:121:TYR:C	1:G:124:TRP:HE1	2.29	0.41
1:G:252:MET:O	1:G:255:SER:HB3	2.22	0.41
1:H:123:GLU:HB3	1:H:125:TYR:CE2	2.56	0.41
1:A:101:THR:OG1	1:A:102:ALA:N	2.54	0.40
1:A:109:ILE:HD13	1:A:109:ILE:HA	1.71	0.40
1:B:30:MET:HE2	1:B:144:ILE:HD12	2.03	0.40
1:C:220:ASP:OD2	1:C:221:LEU:N	2.53	0.40
1:D:278:LEU:HD13	1:D:278:LEU:HA	1.89	0.40
1:E:88:ILE:O	1:E:92:LEU:HG	2.21	0.40
1:E:173:ILE:HD12	1:E:173:ILE:HA	1.61	0.40
1:F:36:VAL:CG1	1:F:146:LEU:CD2	2.99	0.40
1:F:66:ARG:NH1	1:F:67:THR:OG1	2.54	0.40
1:G:68:GLY:HA2	1:G:69:GLY:HA3	1.76	0.40
1:H:173:ILE:HA	1:H:173:ILE:HD12	1.81	0.40
1:A:24:ILE:O	1:A:27:VAL:N	2.54	0.40
1:A:151:VAL:HG11	1:A:227:LEU:HA	2.04	0.40
1:B:36:VAL:HG13	1:B:145:SER:OG	2.21	0.40
1:C:278:LEU:HD13	1:C:278:LEU:HA	1.93	0.40
1:D:142:PHE:HB2	1:D:226:ILE:CD1	2.50	0.40
1:E:275:LEU:O	1:E:278:LEU:N	2.53	0.40
1:F:7:LEU:HB2	1:F:8:PRO:HD3	2.03	0.40
1:G:58:THR:O	1:G:59:LEU:C	2.64	0.40
1:B:96:ALA:C	1:B:98:GLY:H	2.28	0.40
1:E:124:TRP:HA	1:E:127:ILE:HG12	2.02	0.40
1:E:153:VAL:O	1:E:157:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:PHE:CE1	1:G:133:LEU:HD23	2.56	0.40
1:B:69:GLY:CA	1:B:72:PHE:HB3	2.51	0.40
1:E:85:PHE:CE1	1:E:133:LEU:HD23	2.55	0.40
1:F:16:LEU:HD23	1:F:256:LEU:HD23	2.02	0.40
1:G:30:MET:C	1:G:32:ALA:N	2.79	0.40
1:G:259:LEU:HB2	1:G:278:LEU:HD11	2.02	0.40
1:G:270:ASN:HA	1:G:271:PRO:HD2	1.87	0.40
1:H:19:VAL:HG23	1:H:132:VAL:HG22	2.02	0.40
1:H:93:SER:HG	1:H:103:ALA:C	2.29	0.40
1:A:83:MET:O	1:A:86:LEU:HB2	2.20	0.40
1:E:9:LEU:HD23	1:E:9:LEU:HA	1.80	0.40
1:G:107:THR:OG1	1:G:108:LEU:N	2.55	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%)	202 (85%)	26 (11%)	10 (4%)	2	20
1	B	238/301 (79%)	196 (82%)	31 (13%)	11 (5%)	2	19
1	C	238/301 (79%)	201 (84%)	27 (11%)	10 (4%)	2	20
1	D	238/301 (79%)	198 (83%)	29 (12%)	11 (5%)	2	19
1	E	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
1	F	238/301 (79%)	199 (84%)	29 (12%)	10 (4%)	2	20
1	G	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
1	H	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	2	20
All	All	1904/2408 (79%)	1590 (84%)	232 (12%)	82 (4%)	2	20

All (82) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	F	217	GLY
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 ⓘ

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%)	139 (74%)	49 (26%)	0	4
1	B	188/236 (80%)	140 (74%)	48 (26%)	0	4
1	C	188/236 (80%)	137 (73%)	51 (27%)	0	3
1	D	188/236 (80%)	138 (73%)	50 (27%)	0	4
1	E	188/236 (80%)	139 (74%)	49 (26%)	0	4
1	F	188/236 (80%)	135 (72%)	53 (28%)	0	3
1	G	188/236 (80%)	137 (73%)	51 (27%)	0	3
1	H	188/236 (80%)	136 (72%)	52 (28%)	0	3
All	All	1504/1888 (80%)	1101 (73%)	403 (27%)	0	4

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	17	LEU
1	A	35	LEU
1	A	46	ASN
1	A	49	ILE
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	93	SER
1	A	107	THR
1	A	108	LEU
1	A	109	ILE
1	A	115	THR
1	A	119	TYR
1	A	123	GLU
1	A	128	ASP

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Mol	Chain	Res	Type
1	A	129	ILE
1	A	141	ILE
1	A	148	PRO
1	A	149	LEU
1	A	151	VAL
1	A	152	LEU
1	A	153	VAL
1	A	155	LEU
1	A	158	LEU
1	A	168	ARG
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	226	ILE
1	A	227	LEU
1	A	228	VAL
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	252	MET
1	A	257	VAL
1	A	262	LEU
1	A	263	LEU
1	A	266	VAL
1	A	287	LEU
1	A	288	VAL
1	B	10	LEU
1	B	17	LEU
1	B	18	PHE
1	B	46	ASN
1	B	49	ILE
1	B	64	LEU
1	B	66	ARG
1	B	67	THR
1	B	70	ARG
1	B	71	ARG
1	B	77	ILE
1	B	93	SER

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Mol	Chain	Res	Type
1	B	107	THR
1	B	108	LEU
1	B	109	ILE
1	B	115	THR
1	B	119	TYR
1	B	128	ASP
1	B	129	ILE
1	B	141	ILE
1	B	148	PRO
1	B	149	LEU
1	B	151	VAL
1	B	152	LEU
1	B	153	VAL
1	B	155	LEU
1	B	158	LEU
1	B	168	ARG
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
1	B	226	ILE
1	B	228	VAL
1	B	232	HIS
1	B	233	VAL
1	B	234	PHE
1	B	245	SER
1	B	252	MET
1	B	257	VAL
1	B	262	LEU
1	B	263	LEU
1	B	266	VAL
1	B	287	LEU
1	B	288	VAL
1	C	10	LEU
1	C	14	LEU
1	C	17	LEU
1	C	46	ASN
1	C	49	ILE
1	C	64	LEU

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Mol	Chain	Res	Type
1	C	66	ARG
1	C	67	THR
1	C	70	ARG
1	C	71	ARG
1	C	77	ILE
1	C	93	SER
1	C	107	THR
1	C	108	LEU
1	C	109	ILE
1	C	115	THR
1	C	117	LEU
1	C	119	TYR
1	C	123	GLU
1	C	128	ASP
1	C	129	ILE
1	C	141	ILE
1	C	148	PRO
1	C	149	LEU
1	C	151	VAL
1	C	152	LEU
1	C	153	VAL
1	C	155	LEU
1	C	158	LEU
1	C	168	ARG
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	228	VAL
1	C	232	HIS
1	C	233	VAL
1	C	234	PHE
1	C	245	SER
1	C	257	VAL
1	C	262	LEU
1	C	263	LEU
1	C	265	PHE

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Mol	Chain	Res	Type
1	C	266	VAL
1	C	287	LEU
1	C	288	VAL
1	D	10	LEU
1	D	14	LEU
1	D	17	LEU
1	D	18	PHE
1	D	44	VAL
1	D	46	ASN
1	D	49	ILE
1	D	64	LEU
1	D	66	ARG
1	D	67	THR
1	D	70	ARG
1	D	71	ARG
1	D	77	ILE
1	D	93	SER
1	D	107	THR
1	D	108	LEU
1	D	109	ILE
1	D	115	THR
1	D	123	GLU
1	D	128	ASP
1	D	129	ILE
1	D	132	VAL
1	D	141	ILE
1	D	148	PRO
1	D	149	LEU
1	D	151	VAL
1	D	152	LEU
1	D	153	VAL
1	D	155	LEU
1	D	158	LEU
1	D	168	ARG
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	226	ILE

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Mol	Chain	Res	Type
1	D	228	VAL
1	D	232	HIS
1	D	233	VAL
1	D	234	PHE
1	D	245	SER
1	D	257	VAL
1	D	262	LEU
1	D	263	LEU
1	D	266	VAL
1	D	287	LEU
1	D	288	VAL
1	E	14	LEU
1	E	17	LEU
1	E	18	PHE
1	E	46	ASN
1	E	49	ILE
1	E	64	LEU
1	E	66	ARG
1	E	67	THR
1	E	70	ARG
1	E	71	ARG
1	E	77	ILE
1	E	93	SER
1	E	94	LEU
1	E	107	THR
1	E	108	LEU
1	E	109	ILE
1	E	115	THR
1	E	119	TYR
1	E	123	GLU
1	E	128	ASP
1	E	129	ILE
1	E	141	ILE
1	E	148	PRO
1	E	149	LEU
1	E	151	VAL
1	E	152	LEU
1	E	153	VAL
1	E	155	LEU
1	E	158	LEU
1	E	168	ARG
1	E	169	THR

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Mol	Chain	Res	Type
1	E	173	ILE
1	E	174	THR
1	E	175	LEU
1	E	214	PHE
1	E	216	MET
1	E	218	MET
1	E	226	ILE
1	E	228	VAL
1	E	232	HIS
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	266	VAL
1	E	287	LEU
1	E	288	VAL
1	F	10	LEU
1	F	14	LEU
1	F	17	LEU
1	F	18	PHE
1	F	46	ASN
1	F	49	ILE
1	F	58	THR
1	F	64	LEU
1	F	66	ARG
1	F	70	ARG
1	F	71	ARG
1	F	77	ILE
1	F	93	SER
1	F	107	THR
1	F	108	LEU
1	F	109	ILE
1	F	115	THR
1	F	117	LEU
1	F	119	TYR
1	F	123	GLU
1	F	128	ASP
1	F	129	ILE
1	F	141	ILE
1	F	148	PRO

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Mol	Chain	Res	Type
1	F	149	LEU
1	F	151	VAL
1	F	152	LEU
1	F	153	VAL
1	F	155	LEU
1	F	158	LEU
1	F	168	ARG
1	F	169	THR
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	226	ILE
1	F	227	LEU
1	F	228	VAL
1	F	232	HIS
1	F	233	VAL
1	F	234	PHE
1	F	245	SER
1	F	252	MET
1	F	257	VAL
1	F	262	LEU
1	F	263	LEU
1	F	265	PHE
1	F	266	VAL
1	F	287	LEU
1	F	288	VAL
1	G	10	LEU
1	G	14	LEU
1	G	17	LEU
1	G	18	PHE
1	G	46	ASN
1	G	49	ILE
1	G	64	LEU
1	G	66	ARG
1	G	67	THR
1	G	70	ARG
1	G	71	ARG
1	G	77	ILE
1	G	93	SER

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Mol	Chain	Res	Type
1	G	107	THR
1	G	108	LEU
1	G	115	THR
1	G	117	LEU
1	G	119	TYR
1	G	123	GLU
1	G	128	ASP
1	G	129	ILE
1	G	132	VAL
1	G	141	ILE
1	G	148	PRO
1	G	149	LEU
1	G	151	VAL
1	G	152	LEU
1	G	153	VAL
1	G	155	LEU
1	G	158	LEU
1	G	168	ARG
1	G	169	THR
1	G	171	HIS
1	G	173	ILE
1	G	174	THR
1	G	175	LEU
1	G	214	PHE
1	G	216	MET
1	G	218	MET
1	G	226	ILE
1	G	228	VAL
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	266	VAL
1	G	287	LEU
1	G	288	VAL
1	H	10	LEU
1	H	14	LEU
1	H	17	LEU
1	H	18	PHE

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Mol	Chain	Res	Type
1	H	44	VAL
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	77	ILE
1	H	93	SER
1	H	107	THR
1	H	108	LEU
1	H	109	ILE
1	H	115	THR
1	H	117	LEU
1	H	119	TYR
1	H	123	GLU
1	H	128	ASP
1	H	129	ILE
1	H	141	ILE
1	H	148	PRO
1	H	149	LEU
1	H	151	VAL
1	H	152	LEU
1	H	153	VAL
1	H	155	LEU
1	H	158	LEU
1	H	168	ARG
1	H	173	ILE
1	H	174	THR
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	228	VAL
1	H	232	HIS
1	H	233	VAL
1	H	234	PHE
1	H	245	SER
1	H	252	MET

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Mol	Chain	Res	Type
1	H	257	VAL
1	H	262	LEU
1	H	263	LEU
1	H	266	VAL
1	H	287	LEU
1	H	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	272	GLN
1	D	171	HIS
1	E	31	GLN
1	E	279	ASN
1	G	171	HIS
1	G	267	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	246/301 (81%)	0.64	25 (10%)	12	14	81, 117, 188, 281	0
1	B	246/301 (81%)	0.79	33 (13%)	7	10	92, 120, 194, 266	0
1	C	246/301 (81%)	0.73	29 (11%)	9	12	81, 117, 194, 280	0
1	D	246/301 (81%)	0.75	24 (9%)	13	15	99, 124, 189, 250	0
1	E	246/301 (81%)	0.98	37 (15%)	5	9	86, 137, 203, 289	0
1	F	246/301 (81%)	0.86	35 (14%)	6	9	108, 150, 221, 269	0
1	G	246/301 (81%)	0.88	39 (15%)	5	8	83, 126, 197, 287	0
1	H	246/301 (81%)	0.87	35 (14%)	6	9	142, 173, 247, 299	0
All	All	1968/2408 (81%)	0.81	257 (13%)	7	10	81, 133, 210, 299	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	VAL	12.2
1	G	273	ALA	10.7
1	F	232	HIS	10.1
1	H	35	LEU	10.1
1	C	220	ASP	7.8
1	C	232	HIS	7.8
1	G	272	GLN	7.6
1	F	35	LEU	7.4
1	G	179	VAL	7.3
1	G	223	MET	6.7
1	G	166	VAL	6.6
1	E	67	THR	6.4
1	H	232	HIS	6.4
1	H	65	LEU	6.3
1	C	224	PRO	6.2
1	A	36	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	223	MET	6.2
1	D	119	TYR	6.0
1	B	65	LEU	5.9
1	H	34	GLY	5.8
1	F	65	LEU	5.8
1	B	228	VAL	5.7
1	E	36	VAL	5.6
1	E	178	GLY	5.6
1	E	94	LEU	5.3
1	B	266	VAL	5.3
1	H	119	TYR	5.3
1	A	226	ILE	5.3
1	G	220	ASP	5.2
1	H	157	LEU	5.2
1	H	228	VAL	5.2
1	F	228	VAL	5.2
1	C	179	VAL	5.1
1	E	68	GLY	5.0
1	F	81	LEU	5.0
1	C	12	MET	5.0
1	G	262	LEU	4.9
1	E	177	GLU	4.8
1	B	25	VAL	4.8
1	C	262	LEU	4.7
1	E	119	TYR	4.7
1	D	229	VAL	4.6
1	F	9	LEU	4.6
1	H	122	PRO	4.6
1	D	266	VAL	4.5
1	B	119	TYR	4.5
1	B	232	HIS	4.4
1	B	178	GLY	4.4
1	A	65	LEU	4.4
1	H	74	ALA	4.4
1	A	35	LEU	4.4
1	E	95	LEU	4.4
1	G	261	VAL	4.3
1	G	163	ALA	4.3
1	A	179	VAL	4.3
1	G	293	ALA	4.3
1	C	65	LEU	4.3
1	D	232	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	228	VAL	4.2
1	B	27	VAL	4.2
1	D	27	VAL	4.2
1	E	32	ALA	4.2
1	A	261	VAL	4.1
1	E	12	MET	4.0
1	D	227	LEU	4.0
1	G	73	ILE	4.0
1	E	173	ILE	4.0
1	B	229	VAL	3.9
1	B	177	GLU	3.9
1	D	65	LEU	3.9
1	G	265	PHE	3.9
1	E	247	PRO	3.8
1	C	263	LEU	3.8
1	F	264	TYR	3.8
1	E	144	ILE	3.7
1	B	67	THR	3.7
1	F	154	LEU	3.7
1	H	262	LEU	3.7
1	E	166	VAL	3.7
1	B	227	LEU	3.7
1	E	273	ALA	3.7
1	E	127	ILE	3.7
1	G	173	ILE	3.7
1	D	223	MET	3.7
1	H	81	LEU	3.7
1	F	120	LEU	3.6
1	E	142	PHE	3.6
1	B	62	LEU	3.6
1	H	31	GLN	3.6
1	E	214	PHE	3.6
1	H	30	MET	3.6
1	C	120	LEU	3.6
1	C	244	LEU	3.5
1	A	263	LEU	3.5
1	F	62	LEU	3.4
1	G	12	MET	3.4
1	E	99	PRO	3.4
1	E	175	LEU	3.4
1	C	266	VAL	3.4
1	H	179	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	223	MET	3.4
1	A	167	TYR	3.4
1	G	214	PHE	3.4
1	F	36	VAL	3.3
1	F	173	ILE	3.3
1	H	36	VAL	3.3
1	D	73	ILE	3.3
1	B	262	LEU	3.3
1	H	167	TYR	3.3
1	B	220	ASP	3.2
1	G	167	TYR	3.2
1	H	173	ILE	3.2
1	H	286	PHE	3.2
1	D	25	VAL	3.2
1	A	232	HIS	3.2
1	H	161	TYR	3.1
1	A	119	TYR	3.1
1	A	95	LEU	3.1
1	A	17	LEU	3.0
1	A	6	TRP	3.0
1	F	101	THR	3.0
1	A	120	LEU	3.0
1	D	74	ALA	3.0
1	F	158	LEU	3.0
1	H	156	VAL	3.0
1	A	73	ILE	3.0
1	E	280	GLY	3.0
1	F	82	PHE	2.9
1	C	167	TYR	2.9
1	C	221	LEU	2.9
1	D	95	LEU	2.9
1	G	232	HIS	2.9
1	G	263	LEU	2.9
1	E	279	ASN	2.9
1	D	62	LEU	2.8
1	H	71	ARG	2.8
1	E	233	VAL	2.8
1	H	244	LEU	2.8
1	E	14	LEU	2.8
1	G	178	GLY	2.8
1	A	223	MET	2.8
1	H	287	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	124	TRP	2.8
1	D	179	VAL	2.8
1	D	233	VAL	2.8
1	C	11	GLY	2.8
1	C	176	ALA	2.7
1	H	62	LEU	2.7
1	B	225	SER	2.7
1	D	82	PHE	2.7
1	D	269	GLY	2.7
1	G	222	ILE	2.7
1	G	254	GLY	2.7
1	G	82	PHE	2.6
1	G	251	ALA	2.6
1	A	25	VAL	2.6
1	B	60	VAL	2.6
1	F	149	LEU	2.6
1	H	144	ILE	2.6
1	B	26	LEU	2.6
1	F	157	LEU	2.6
1	H	28	MET	2.6
1	F	41	PRO	2.6
1	A	262	LEU	2.5
1	C	79	PHE	2.5
1	C	73	ILE	2.5
1	F	124	TRP	2.5
1	H	221	LEU	2.5
1	B	61	LEU	2.5
1	A	144	ILE	2.5
1	E	73	ILE	2.5
1	A	131	GLY	2.5
1	B	68	GLY	2.5
1	E	34	GLY	2.5
1	B	23	ALA	2.5
1	F	134	ILE	2.5
1	B	6	TRP	2.4
1	A	245	SER	2.4
1	F	30	MET	2.4
1	H	223	MET	2.4
1	G	158	LEU	2.4
1	B	233	VAL	2.4
1	E	138	VAL	2.4
1	F	79	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	259	LEU	2.4
1	G	175	LEU	2.4
1	G	282	ALA	2.4
1	C	41	PRO	2.4
1	C	166	VAL	2.4
1	C	234	PHE	2.4
1	H	124	TRP	2.4
1	A	22	ILE	2.3
1	F	28	MET	2.3
1	B	95	LEU	2.3
1	G	224	PRO	2.3
1	C	9	LEU	2.3
1	F	8	PRO	2.3
1	A	27	VAL	2.3
1	G	124	TRP	2.3
1	H	168	ARG	2.3
1	D	259	LEU	2.3
1	G	127	ILE	2.3
1	C	178	GLY	2.3
1	G	153	VAL	2.3
1	B	28	MET	2.3
1	F	34	GLY	2.3
1	F	164	ILE	2.2
1	C	158	LEU	2.2
1	E	65	LEU	2.2
1	F	5	ASP	2.2
1	B	105	ALA	2.2
1	H	158	LEU	2.2
1	E	220	ASP	2.2
1	B	253	VAL	2.2
1	F	175	LEU	2.2
1	G	150	PRO	2.2
1	G	274	GLY	2.2
1	B	179	VAL	2.2
1	F	172	MET	2.2
1	F	223	MET	2.2
1	E	161	TYR	2.2
1	F	161	TYR	2.2
1	B	24	ILE	2.2
1	A	79	PHE	2.2
1	F	57	PHE	2.2
1	G	79	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	247	PRO	2.2
1	A	62	LEU	2.1
1	E	15	MET	2.1
1	E	249	LEU	2.1
1	F	119	TYR	2.1
1	F	167	TYR	2.1
1	G	119	TYR	2.1
1	E	69	GLY	2.1
1	F	99	PRO	2.1
1	B	57	PHE	2.1
1	G	50	PHE	2.1
1	H	138	VAL	2.1
1	C	124	TRP	2.1
1	G	162	ASP	2.1
1	H	70	ARG	2.1
1	C	255	SER	2.1
1	C	227	LEU	2.1
1	G	152	LEU	2.1
1	H	164	ILE	2.1
1	B	255	SER	2.1
1	H	227	LEU	2.1
1	E	176	ALA	2.0
1	G	76	PHE	2.0
1	D	12	MET	2.0
1	C	133	LEU	2.0
1	B	112	VAL	2.0
1	D	36	VAL	2.0
1	D	60	VAL	2.0
1	E	254	GLY	2.0
1	E	281	GLY	2.0
1	D	220	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.