



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 PM UTC

PDB ID : 1ST6 / pdb_00001st6
Title : Crystal structure of a cytoskeletal protein
Authors : Bakolitsa, C.; Liddington, R.C.
Deposited on : 2004-03-25
Resolution : 3.10 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

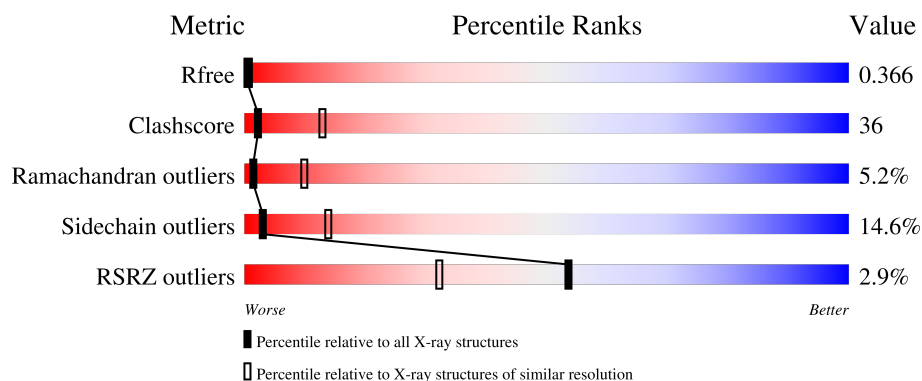
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1069	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8058 atoms, of which 3 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 Vinculin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1049	Total	C	H	N	O	S	0	0	0
			8058	4978	3	1460	1568	49			

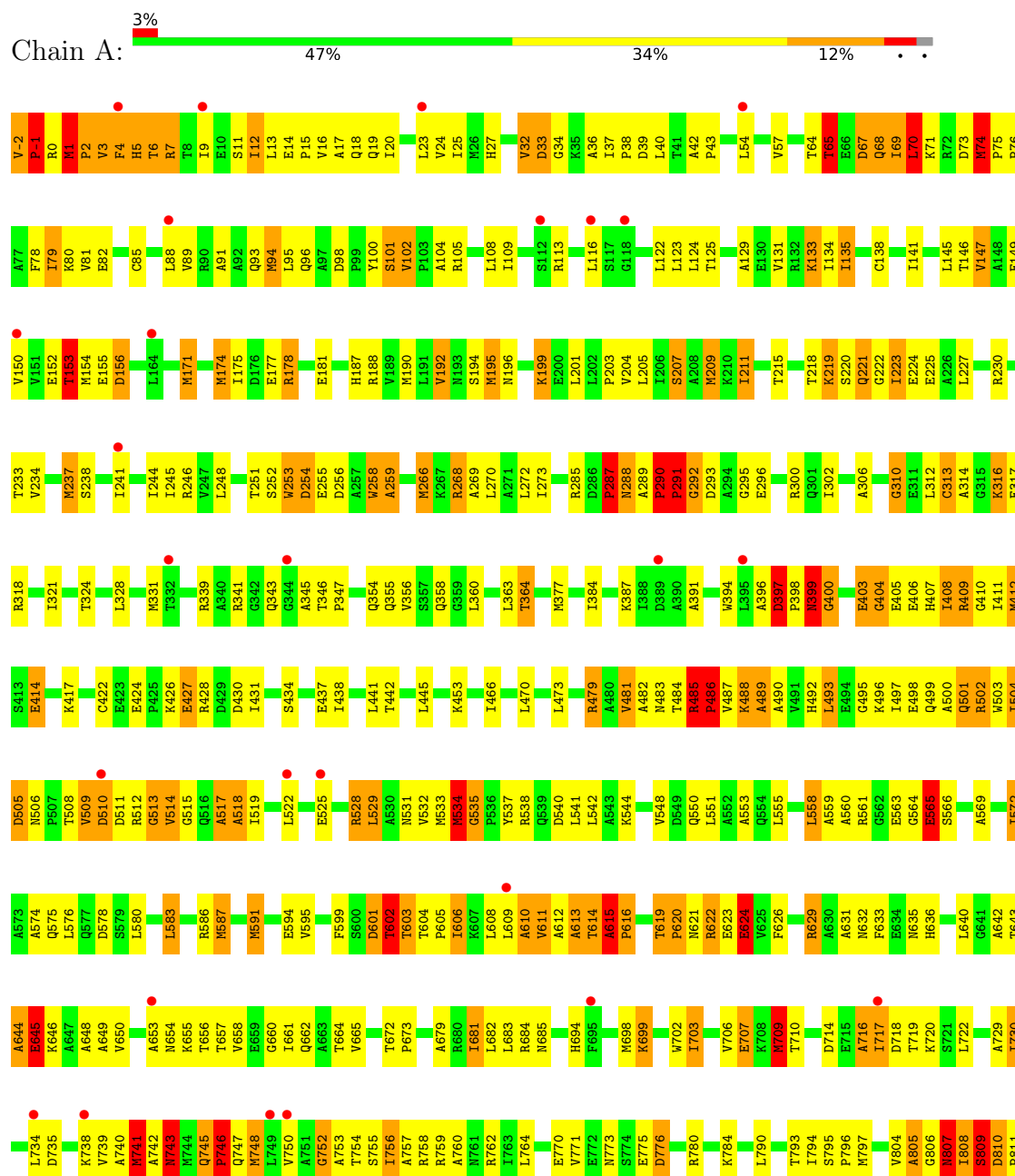
There are 4 discrepancies between the modelled and reference sequences:

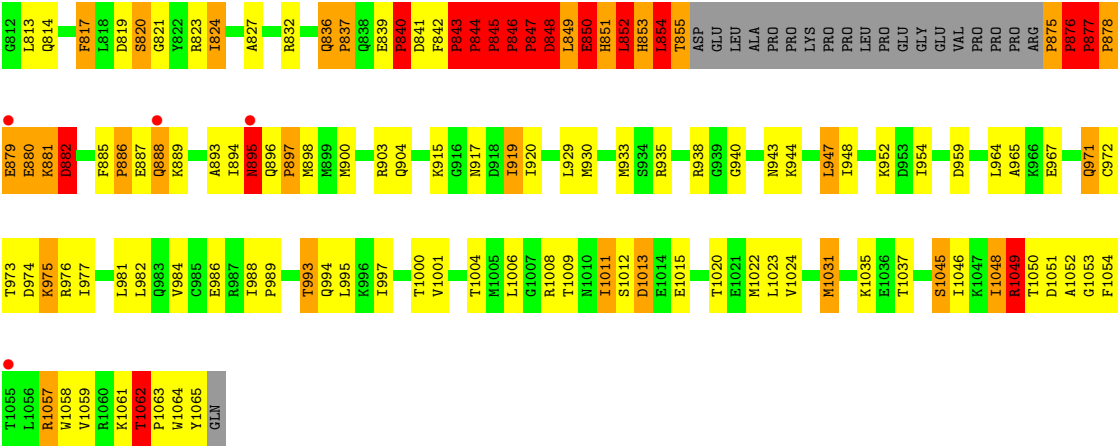
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	VAL	-	cloning artifact	UNP P12003
A	-1	PRO	-	cloning artifact	UNP P12003
A	0	ARG	-	cloning artifact	UNP P12003
A	1	MET	-	initiating methionine	UNP P12003

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: Vinculin





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	56.02Å 126.95Å 351.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.10 46.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.96-3.10) 99.9 (46.96-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.316 , 0.357 0.320 , 0.366	Depositor DCC
R_{free} test set	1134 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	102.2	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8058	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [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	1.09	47/8154 (0.6%)	1.53	193/11006 (1.8%)

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	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	PRO	N-CD	23.33	1.80	1.47
1	A	-1	PRO	N-CA	21.14	1.74	1.47
1	A	-1	PRO	CA-CB	-15.63	1.31	1.53
1	A	613	ALA	CA-CB	-15.18	1.26	1.53
1	A	709	MET	SD-CE	-10.25	1.53	1.79
1	A	74	MET	SD-CE	10.15	2.04	1.79
1	A	291	PRO	CA-C	-9.87	1.38	1.52
1	A	876	PRO	CA-C	9.79	1.61	1.52
1	A	875	PRO	N-CD	9.66	1.61	1.47
1	A	190	MET	SD-CE	-9.37	1.56	1.79
1	A	877	PRO	CA-C	8.86	1.60	1.52
1	A	836	GLN	CA-C	8.84	1.64	1.52
1	A	611	VAL	CA-CB	8.80	1.65	1.54
1	A	853	HIS	CB-CG	8.63	1.62	1.50
1	A	844	PRO	CA-C	8.25	1.59	1.52
1	A	174	MET	SD-CE	-7.87	1.59	1.79
1	A	-1	PRO	CA-C	7.72	1.63	1.52
1	A	875	PRO	CA-C	-7.67	1.36	1.52
1	A	203	PRO	CA-C	-7.27	1.41	1.52
1	A	645	GLU	CB-CG	6.95	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	THR	CA-C	6.83	1.61	1.52
1	A	409	ARG	N-CA	-6.77	1.38	1.46
1	A	1031	MET	SD-CE	-6.76	1.62	1.79
1	A	718	ASP	CA-C	-6.74	1.44	1.52
1	A	854	LEU	N-CA	6.55	1.54	1.46
1	A	293	ASP	N-CA	-6.30	1.39	1.46
1	A	718	ASP	N-CA	6.27	1.53	1.46
1	A	718	ASP	CB-CG	6.26	1.67	1.52
1	A	854	LEU	CA-C	-6.13	1.44	1.52
1	A	601	ASP	CA-C	-6.13	1.44	1.52
1	A	612	ALA	CA-CB	-6.11	1.43	1.53
1	A	412	MET	SD-CE	-6.09	1.64	1.79
1	A	293	ASP	CA-CB	-6.07	1.44	1.53
1	A	331	MET	SD-CE	5.97	1.94	1.79
1	A	195	MET	SD-CE	-5.91	1.64	1.79
1	A	266	MET	SD-CE	-5.72	1.65	1.79
1	A	611	VAL	CA-C	-5.66	1.44	1.52
1	A	192	VAL	CA-CB	-5.60	1.46	1.54
1	A	845	PRO	CA-C	5.56	1.57	1.52
1	A	603	THR	N-CA	5.54	1.53	1.46
1	A	591	MET	SD-CE	5.48	1.93	1.79
1	A	-2	VAL	C-N	5.45	1.46	1.33
1	A	587	MET	SD-CE	-5.43	1.66	1.79
1	A	645	GLU	N-CA	5.37	1.53	1.46
1	A	876	PRO	C-N	5.27	1.39	1.33
1	A	645	GLU	CA-CB	5.26	1.61	1.53
1	A	408	ILE	CA-C	-5.07	1.45	1.52

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-1	PRO	N-CA-CB	19.62	123.86	103.25
1	A	-1	PRO	CA-N-CD	-19.49	84.71	112.00
1	A	876	PRO	N-CA-C	18.42	133.17	110.70
1	A	-2	VAL	C-N-CD	-16.91	55.68	125.00
1	A	877	PRO	N-CA-C	14.82	128.78	110.70
1	A	290	PRO	N-CA-C	13.95	127.72	110.70
1	A	852	LEU	CA-C-N	-13.85	101.73	122.23
1	A	852	LEU	C-N-CA	-13.85	101.73	122.23
1	A	611	VAL	CA-C-N	-12.65	103.42	120.63
1	A	611	VAL	C-N-CA	-12.65	103.42	120.63
1	A	565	GLU	N-CA-C	-12.34	84.53	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	741	MET	N-CA-C	11.43	124.86	111.71
1	A	485	ARG	N-CA-C	11.38	134.97	109.81
1	A	-2	VAL	O-C-N	11.23	140.97	123.00
1	A	614	THR	N-CA-C	-11.12	98.01	111.69
1	A	-1	PRO	N-CA-C	-10.91	89.99	112.47
1	A	843	PRO	CA-N-CD	-10.88	96.77	112.00
1	A	518	ALA	N-CA-C	-10.59	98.66	111.69
1	A	809	SER	N-CA-C	10.51	133.19	110.80
1	A	645	GLU	N-CA-CB	10.45	126.31	110.22
1	A	748	MET	N-CA-C	-10.42	100.68	113.50
1	A	684	ARG	N-CA-C	-10.31	100.23	113.12
1	A	564	GLY	CA-C-N	10.28	141.17	121.54
1	A	564	GLY	C-N-CA	10.28	141.17	121.54
1	A	291	PRO	N-CA-C	10.27	133.63	112.47
1	A	289	ALA	N-CA-C	-9.95	88.41	109.01
1	A	845	PRO	CA-N-CD	-9.48	98.72	112.00
1	A	851	HIS	CA-C-N	-9.45	109.28	123.07
1	A	851	HIS	C-N-CA	-9.45	109.28	123.07
1	A	487	VAL	N-CA-C	-9.44	94.95	108.17
1	A	32	VAL	N-CA-C	9.13	120.95	111.00
1	A	844	PRO	CA-N-CD	-8.93	99.49	112.00
1	A	290	PRO	CA-C-N	8.80	130.84	119.84
1	A	290	PRO	C-N-CA	8.80	130.84	119.84
1	A	486	PRO	CA-N-CD	-8.65	99.89	112.00
1	A	513	GLY	N-CA-C	-8.56	92.88	113.18
1	A	854	LEU	CB-CA-C	-8.54	93.43	110.42
1	A	409	ARG	N-CA-C	-8.51	102.08	111.36
1	A	427	GLU	N-CA-C	-8.48	102.95	113.38
1	A	847	PRO	CA-N-CD	-8.48	100.13	112.00
1	A	807	ASN	N-CA-CB	-8.47	97.23	109.85
1	A	844	PRO	N-CA-C	8.46	121.03	110.70
1	A	602	THR	CA-C-N	8.37	137.53	121.54
1	A	602	THR	C-N-CA	8.37	137.53	121.54
1	A	2	PRO	CA-N-CD	-8.34	100.33	112.00
1	A	880	GLU	N-CA-C	8.22	122.86	108.56
1	A	489	ALA	N-CA-C	8.18	128.21	110.80
1	A	534	MET	N-CA-C	8.15	123.05	110.42
1	A	1049	ARG	N-CA-C	8.08	122.44	110.48
1	A	849	LEU	CA-C-N	8.05	136.91	121.54
1	A	849	LEU	C-N-CA	8.05	136.91	121.54
1	A	293	ASP	CA-CB-CG	-7.99	104.61	112.60
1	A	850	GLU	CB-CG-CD	7.89	126.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	PRO	CA-N-CD	-7.86	101.00	112.00
1	A	519	ILE	N-CA-C	-7.63	102.84	110.62
1	A	718	ASP	N-CA-CB	7.59	120.88	109.19
1	A	223	ILE	N-CA-C	-7.47	103.67	111.58
1	A	846	PRO	N-CA-C	7.41	119.74	110.70
1	A	603	THR	N-CA-C	7.25	126.25	110.80
1	A	601	ASP	N-CA-C	7.19	119.20	111.36
1	A	65	THR	N-CA-C	-7.15	101.09	110.53
1	A	5	HIS	N-CA-C	7.09	121.96	113.16
1	A	517	ALA	N-CA-C	-7.06	103.84	113.30
1	A	512	ARG	N-CA-C	7.05	120.60	109.39
1	A	3	VAL	N-CA-C	7.04	118.42	108.36
1	A	566	SER	N-CA-C	-7.01	100.11	110.20
1	A	560	ALA	N-CA-C	-7.00	104.90	113.50
1	A	707	GLU	N-CA-C	-6.98	103.75	111.36
1	A	806	GLY	N-CA-C	-6.98	96.63	113.18
1	A	876	PRO	CA-C-N	6.98	127.57	120.38
1	A	876	PRO	C-N-CA	6.98	127.57	120.38
1	A	848	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	290	PRO	CB-CA-C	6.72	119.12	110.92
1	A	428	ARG	N-CA-C	-6.69	104.07	111.36
1	A	610	ALA	CA-C-N	-6.64	109.75	120.64
1	A	610	ALA	C-N-CA	-6.64	109.75	120.64
1	A	417	LYS	N-CA-C	-6.61	104.16	111.36
1	A	253	TRP	N-CA-C	-6.59	100.45	110.14
1	A	397	ASP	N-CA-C	6.59	124.37	109.81
1	A	806	GLY	CA-C-N	6.58	130.16	120.95
1	A	806	GLY	C-N-CA	6.58	130.16	120.95
1	A	153	THR	N-CA-C	6.52	120.67	110.17
1	A	408	ILE	CB-CA-C	-6.49	103.42	111.92
1	A	113	ARG	N-CA-C	-6.48	104.85	112.89
1	A	133	LYS	N-CA-C	-6.47	104.31	111.36
1	A	1	MET	N-CA-C	6.45	124.06	109.81
1	A	823	ARG	N-CA-C	-6.44	104.91	112.89
1	A	171	MET	N-CA-C	-6.38	104.98	112.89
1	A	404	GLY	CA-C-O	6.38	129.35	119.15
1	A	717	ILE	CB-CA-C	6.37	120.35	112.45
1	A	886	PRO	N-CA-C	6.37	120.43	111.33
1	A	645	GLU	CB-CG-CD	6.36	123.42	112.60
1	A	187	HIS	N-CA-C	-6.33	105.04	112.89
1	A	849	LEU	CB-CA-C	-6.32	102.44	112.05
1	A	819	ASP	N-CA-C	-6.28	104.67	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASP	N-CA-CB	6.26	120.67	110.90
1	A	473	LEU	N-CA-C	-6.26	104.70	112.90
1	A	611	VAL	N-CA-CB	6.26	125.39	111.50
1	A	11	SER	CA-C-N	-6.25	116.59	122.66
1	A	11	SER	C-N-CA	-6.25	116.59	122.66
1	A	18	GLN	N-CA-C	-6.16	104.46	112.23
1	A	328	LEU	N-CA-C	-6.10	105.88	113.38
1	A	846	PRO	CB-CA-C	6.05	118.30	110.92
1	A	877	PRO	CA-C-N	6.04	127.39	119.84
1	A	877	PRO	C-N-CA	6.04	127.39	119.84
1	A	717	ILE	N-CA-CB	-6.03	105.62	111.89
1	A	959	ASP	N-CA-C	-6.03	104.83	111.82
1	A	203	PRO	CA-N-CD	-6.02	103.57	112.00
1	A	355	GLN	N-CA-C	-6.00	105.96	113.28
1	A	437	GLU	N-CA-C	-5.99	105.46	112.89
1	A	875	PRO	N-CA-C	5.99	127.07	112.10
1	A	840	PRO	CA-N-CD	-5.96	103.65	112.00
1	A	78	PHE	N-CA-C	-5.95	105.51	112.89
1	A	253	TRP	CA-C-N	5.93	132.15	122.07
1	A	253	TRP	C-N-CA	5.93	132.15	122.07
1	A	827	ALA	N-CA-C	-5.89	104.81	112.23
1	A	254	ASP	N-CA-C	5.89	118.05	108.63
1	A	1	MET	C-N-CD	-5.86	100.96	125.00
1	A	919	ILE	N-CA-C	-5.83	105.05	110.53
1	A	145	LEU	N-CA-C	-5.81	106.02	113.23
1	A	291	PRO	CA-N-CD	-5.81	103.86	112.00
1	A	852	LEU	N-CA-C	5.79	118.14	108.02
1	A	535	GLY	N-CA-C	5.77	124.11	112.34
1	A	603	THR	CB-CA-C	-5.74	98.99	110.42
1	A	730	ILE	N-CA-C	-5.74	104.74	111.00
1	A	364	THR	N-CA-C	-5.73	105.01	112.23
1	A	629	ARG	N-CA-C	-5.71	105.42	112.90
1	A	254	ASP	CB-CA-C	-5.67	101.80	110.88
1	A	293	ASP	N-CA-C	5.66	117.60	107.80
1	A	611	VAL	N-CA-C	-5.66	104.63	112.50
1	A	74	MET	CA-C-N	-5.66	114.55	120.38
1	A	74	MET	C-N-CA	-5.66	114.55	120.38
1	A	292	GLY	CA-C-N	-5.66	114.24	122.44
1	A	292	GLY	C-N-CA	-5.66	114.24	122.44
1	A	895	ASN	N-CA-C	5.65	122.83	110.80
1	A	252	SER	CA-C-N	-5.65	112.94	123.05
1	A	252	SER	C-N-CA	-5.65	112.94	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	LYS	CA-C-N	5.63	132.30	121.54
1	A	488	LYS	C-N-CA	5.63	132.30	121.54
1	A	482	ALA	N-CA-C	5.63	118.27	111.40
1	A	875	PRO	CB-CA-C	5.61	120.76	110.10
1	A	993	THR	N-CA-C	-5.61	105.93	112.89
1	A	1013	ASP	N-CA-C	5.55	119.55	112.34
1	A	259	ALA	N-CA-C	5.52	116.98	111.07
1	A	310	GLY	N-CA-C	5.52	119.57	112.83
1	A	1046	ILE	N-CA-C	-5.50	106.33	111.45
1	A	824	ILE	N-CA-C	-5.47	105.76	110.74
1	A	752	GLY	N-CA-C	-5.45	107.90	114.66
1	A	716	ALA	CA-C-N	-5.43	116.61	122.59
1	A	716	ALA	C-N-CA	-5.43	116.61	122.59
1	A	485	ARG	C-N-CD	-5.42	102.77	125.00
1	A	564	GLY	O-C-N	5.41	129.73	122.70
1	A	293	ASP	CB-CA-C	-5.40	102.73	110.62
1	A	965	ALA	N-CA-C	-5.40	105.42	112.23
1	A	837	PRO	CA-N-CD	-5.40	104.44	112.00
1	A	70	LEU	N-CA-C	-5.37	105.46	112.23
1	A	885	PHE	CA-C-N	5.37	126.12	120.11
1	A	885	PHE	C-N-CA	5.37	126.12	120.11
1	A	740	ALA	N-CA-C	-5.33	106.80	113.15
1	A	947	LEU	N-CA-C	-5.33	105.51	112.23
1	A	12	ILE	N-CA-C	-5.33	107.59	111.90
1	A	853	HIS	CA-CB-CG	5.32	119.12	113.80
1	A	820	SER	N-CA-C	-5.32	106.63	113.23
1	A	645	GLU	N-CA-C	-5.31	105.60	111.71
1	A	853	HIS	CB-CG-ND1	5.31	130.66	122.70
1	A	266	MET	N-CA-C	-5.29	105.59	111.36
1	A	312	LEU	N-CA-C	-5.29	105.11	112.30
1	A	615	ALA	N-CA-C	5.28	121.49	109.81
1	A	306	ALA	N-CA-C	-5.24	106.40	112.89
1	A	509	VAL	N-CA-C	5.24	117.94	110.09
1	A	178	ARG	N-CA-C	5.23	116.67	110.97
1	A	644	ALA	CA-C-O	-5.23	115.31	120.80
1	A	488	LYS	N-CA-C	5.23	118.24	110.14
1	A	409	ARG	CB-CA-C	5.23	119.73	110.85
1	A	599	PHE	N-CA-C	5.21	119.28	113.02
1	A	316	LYS	N-CA-C	-5.20	105.22	112.45
1	A	479	ARG	N-CA-C	-5.18	106.74	113.16
1	A	493	LEU	N-CA-C	5.14	116.70	111.14
1	A	269	ALA	N-CA-C	-5.14	106.17	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	995	LEU	N-CA-C	-5.13	106.86	113.23
1	A	644	ALA	CA-C-N	-5.12	112.90	120.28
1	A	644	ALA	C-N-CA	-5.12	112.90	120.28
1	A	846	PRO	N-CA-CB	-5.12	98.11	103.08
1	A	898	MET	N-CA-C	-5.07	105.94	111.82
1	A	784	LYS	N-CA-C	-5.06	106.61	112.89
1	A	681	ILE	CB-CA-C	-5.06	105.24	112.22
1	A	897	PRO	N-CA-C	-5.05	108.03	114.35
1	A	952	LYS	N-CA-C	-5.05	106.96	113.23
1	A	632	ASN	N-CA-C	-5.04	106.98	113.23
1	A	776	ASP	CA-C-N	5.04	126.14	119.84
1	A	776	ASP	C-N-CA	5.04	126.14	119.84
1	A	840	PRO	CA-CB-CG	-5.04	94.93	104.50
1	A	203	PRO	O-C-N	5.02	128.25	122.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8055	3	8219	594	1
All	All	8055	3	8219	594	1

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 36.

All (594) 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:613:ALA:HB3	1:A:683:LEU:CD1	1.35	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:PRO:N	1:A:-1:PRO:CA	1.74	1.49
1:A:74:MET:SD	1:A:74:MET:CE	2.04	1.45
1:A:391:ALA:CB	1:A:407:HIS:HB3	1.54	1.37
1:A:613:ALA:CB	1:A:683:LEU:HD13	1.54	1.36
1:A:149:GLU:HG3	1:A:230:ARG:CZ	1.56	1.33
1:A:845:PRO:O	1:A:847:PRO:HD3	1.29	1.25
1:A:613:ALA:CB	1:A:683:LEU:CG	2.17	1.23
1:A:613:ALA:CB	1:A:683:LEU:CD1	2.14	1.21
1:A:613:ALA:CB	1:A:683:LEU:HD22	1.71	1.20
1:A:613:ALA:HB1	1:A:683:LEU:CD2	1.72	1.20
1:A:756:ILE:CG1	1:A:797:MET:HE1	1.72	1.20
1:A:0:ARG:O	1:A:1:MET:HG2	1.42	1.18
1:A:613:ALA:CB	1:A:683:LEU:HB3	1.73	1.18
1:A:268:ARG:NH2	1:A:645:GLU:OE1	1.73	1.18
1:A:138:CYS:HA	1:A:141:ILE:HD12	1.17	1.16
1:A:613:ALA:CB	1:A:683:LEU:CD2	2.27	1.12
1:A:149:GLU:HG3	1:A:230:ARG:NH1	1.64	1.12
1:A:391:ALA:HB2	1:A:407:HIS:HB3	1.19	1.11
1:A:613:ALA:HB1	1:A:683:LEU:HD22	1.23	1.11
1:A:613:ALA:CB	1:A:683:LEU:CB	2.30	1.10
1:A:490:ALA:HB1	1:A:496:LYS:HE2	1.20	1.09
1:A:504:ILE:HG13	1:A:576:LEU:HD23	1.35	1.09
1:A:845:PRO:O	1:A:847:PRO:CD	2.02	1.08
1:A:1045:SER:O	1:A:1048:ILE:HD11	1.52	1.07
1:A:613:ALA:HB2	1:A:683:LEU:HB3	1.32	1.07
1:A:613:ALA:HB3	1:A:683:LEU:CG	1.83	1.06
1:A:387:LYS:HB2	1:A:411:ILE:HD11	1.08	1.05
1:A:314:ALA:HA	1:A:485:ARG:HG2	1.35	1.05
1:A:756:ILE:HG13	1:A:797:MET:HE1	1.38	1.04
1:A:391:ALA:HB1	1:A:407:HIS:HB3	1.35	1.04
1:A:756:ILE:CB	1:A:797:MET:HE1	1.88	1.04
1:A:699:LYS:O	1:A:703:ILE:HD13	1.58	1.03
1:A:613:ALA:C	1:A:683:LEU:HD22	1.84	1.03
1:A:504:ILE:HG13	1:A:576:LEU:CD2	1.89	1.02
1:A:851:HIS:O	1:A:852:LEU:CD1	2.09	1.00
1:A:752:GLY:O	1:A:756:ILE:HD13	1.62	0.99
1:A:559:ALA:HB2	1:A:563:GLU:O	1.63	0.98
1:A:0:ARG:O	1:A:1:MET:CG	2.11	0.97
1:A:844:PRO:C	1:A:846:PRO:HD2	1.90	0.97
1:A:930:MET:HE3	1:A:930:MET:HA	1.44	0.97
1:A:391:ALA:CB	1:A:407:HIS:CB	2.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ALA:HB1	1:A:683:LEU:CB	1.93	0.97
1:A:149:GLU:CG	1:A:230:ARG:CZ	2.42	0.95
1:A:605:PRO:HB3	1:A:633:PHE:HD1	1.26	0.95
1:A:613:ALA:HB1	1:A:683:LEU:CG	1.92	0.95
1:A:605:PRO:CB	1:A:633:PHE:HD1	1.80	0.95
1:A:285:ARG:O	1:A:287:PRO:HD3	1.68	0.94
1:A:741:MET:CE	1:A:817:PHE:CE2	2.51	0.94
1:A:74:MET:HE2	1:A:122:LEU:CD1	1.98	0.93
1:A:653:ALA:O	1:A:657:THR:HB	1.68	0.93
1:A:314:ALA:CA	1:A:485:ARG:HG2	1.98	0.93
1:A:741:MET:SD	1:A:817:PHE:HE2	1.91	0.92
1:A:753:ALA:HA	1:A:756:ILE:HD11	1.52	0.92
1:A:606:ILE:HD13	1:A:606:ILE:H	1.34	0.91
1:A:741:MET:SD	1:A:817:PHE:CE2	2.63	0.91
1:A:851:HIS:O	1:A:852:LEU:HD12	1.68	0.91
1:A:116:LEU:HD13	1:A:1001:VAL:HG22	1.51	0.90
1:A:738:LYS:HZ2	1:A:817:PHE:HE1	0.91	0.90
1:A:149:GLU:HG3	1:A:230:ARG:NH2	1.85	0.89
1:A:756:ILE:HB	1:A:797:MET:HE1	1.52	0.89
1:A:613:ALA:HB3	1:A:683:LEU:HD13	0.88	0.88
1:A:973:THR:HG21	1:A:1049:ARG:CG	2.04	0.88
1:A:514:VAL:HB	1:A:517:ALA:HB3	1.57	0.87
1:A:591:MET:SD	1:A:717:ILE:HG13	2.14	0.87
1:A:525:GLU:O	1:A:529:LEU:HG	1.74	0.87
1:A:611:VAL:O	1:A:615:ALA:HB3	1.74	0.87
1:A:795:SER:HB3	1:A:796:PRO:HD3	1.58	0.86
1:A:613:ALA:HB1	1:A:683:LEU:HB3	1.54	0.86
1:A:-2:VAL:HG12	1:A:-1:PRO:N	1.91	0.85
1:A:-2:VAL:CG1	1:A:-1:PRO:N	2.39	0.85
1:A:391:ALA:HB2	1:A:407:HIS:CB	2.03	0.85
1:A:603:THR:HA	1:A:606:ILE:HD11	1.59	0.85
1:A:930:MET:HE1	1:A:933:MET:SD	2.17	0.85
1:A:734:LEU:HB3	1:A:738:LYS:HE2	1.60	0.84
1:A:605:PRO:HB3	1:A:633:PHE:CD1	2.12	0.84
1:A:973:THR:CG2	1:A:1049:ARG:HG3	2.07	0.84
1:A:74:MET:CE	1:A:122:LEU:CD1	2.55	0.84
1:A:504:ILE:HG23	1:A:505:ASP:N	1.94	0.83
1:A:314:ALA:HA	1:A:485:ARG:CG	2.08	0.83
1:A:851:HIS:O	1:A:852:LEU:HD13	1.76	0.83
1:A:387:LYS:CB	1:A:411:ILE:HD11	2.02	0.82
1:A:528:ARG:CG	1:A:529:LEU:HD23	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:PRO:N	1:A:-1:PRO:C	2.38	0.81
1:A:529:LEU:HD23	1:A:529:LEU:N	1.94	0.81
1:A:74:MET:HE2	1:A:122:LEU:HD11	1.61	0.81
1:A:285:ARG:O	1:A:287:PRO:CD	2.29	0.81
1:A:971:GLN:HA	1:A:1049:ARG:HH21	1.44	0.80
1:A:734:LEU:HD22	1:A:738:LYS:HZ3	1.46	0.79
1:A:738:LYS:O	1:A:741:MET:HB2	1.81	0.79
1:A:138:CYS:HA	1:A:141:ILE:CD1	2.07	0.79
1:A:613:ALA:CA	1:A:683:LEU:HD22	2.12	0.79
1:A:74:MET:CE	1:A:122:LEU:HD11	2.14	0.78
1:A:974:ASP:OD2	1:A:976:ARG:HG2	1.84	0.78
1:A:504:ILE:CG1	1:A:576:LEU:HD23	2.12	0.78
1:A:896:GLN:N	1:A:897:PRO:HD3	1.99	0.78
1:A:613:ALA:O	1:A:683:LEU:HD22	1.84	0.78
1:A:407:HIS:O	1:A:411:ILE:HG12	1.83	0.77
1:A:971:GLN:HA	1:A:1049:ARG:NH2	2.00	0.77
1:A:756:ILE:HG13	1:A:797:MET:CE	2.15	0.77
1:A:138:CYS:CA	1:A:141:ILE:HD12	2.09	0.76
1:A:976:ARG:HG3	1:A:977:ILE:N	2.01	0.76
1:A:314:ALA:HB3	1:A:317:GLU:HB3	1.67	0.76
1:A:408:ILE:O	1:A:412:MET:HG3	1.86	0.75
1:A:504:ILE:HG23	1:A:505:ASP:H	1.51	0.75
1:A:738:LYS:NZ	1:A:817:PHE:HE1	1.80	0.75
1:A:742:ALA:O	1:A:745:GLN:NE2	2.20	0.75
1:A:391:ALA:HB1	1:A:407:HIS:CB	2.11	0.75
1:A:605:PRO:CB	1:A:633:PHE:CD1	2.67	0.74
1:A:808:ILE:N	1:A:813:LEU:HD11	2.02	0.74
1:A:74:MET:CE	1:A:122:LEU:HD12	2.18	0.74
1:A:9:ILE:HD12	1:A:123:LEU:HB3	1.69	0.74
1:A:141:ILE:HD13	1:A:171:MET:SD	2.28	0.74
1:A:408:ILE:HG22	1:A:412:MET:SD	2.29	0.73
1:A:881:LYS:HZ2	1:A:915:LYS:HG2	1.53	0.73
1:A:614:THR:O	1:A:616:PRO:CD	2.37	0.73
1:A:0:ARG:C	1:A:1:MET:HG2	2.13	0.73
1:A:149:GLU:CG	1:A:230:ARG:NH2	2.51	0.73
1:A:69:ILE:HD13	1:A:69:ILE:H	1.52	0.73
1:A:613:ALA:HB3	1:A:683:LEU:CD2	2.09	0.73
1:A:973:THR:HG21	1:A:1049:ARG:HG3	1.65	0.73
1:A:853:HIS:O	1:A:854:LEU:HG	1.89	0.72
1:A:845:PRO:N	1:A:846:PRO:HD2	2.04	0.72
1:A:3:VAL:C	1:A:4:PHE:HD2	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ILE:O	1:A:813:LEU:HG	1.89	0.72
1:A:196:ASN:HA	1:A:199:LYS:HD3	1.72	0.72
1:A:255:GLU:O	1:A:258:TRP:CE3	2.42	0.72
1:A:702:TRP:HE3	1:A:703:ILE:HD12	1.55	0.72
1:A:559:ALA:CB	1:A:563:GLU:O	2.38	0.72
1:A:993:THR:O	1:A:997:ILE:HD13	1.89	0.72
1:A:490:ALA:CB	1:A:496:LYS:HE2	2.11	0.71
1:A:845:PRO:N	1:A:846:PRO:CD	2.53	0.71
1:A:528:ARG:HG3	1:A:529:LEU:HD23	1.72	0.71
1:A:613:ALA:HB2	1:A:683:LEU:HD13	1.65	0.71
1:A:406:GLU:O	1:A:410:GLY:HA3	1.91	0.71
1:A:503:TRP:CD1	1:A:515:GLY:HA3	2.26	0.71
1:A:729:ALA:HB3	1:A:759:ARG:HH22	1.55	0.70
1:A:747:GLN:HE22	1:A:750:VAL:HG21	1.55	0.70
1:A:109:ILE:HD11	1:A:1004:THR:HA	1.73	0.70
1:A:9:ILE:CD1	1:A:123:LEU:HD22	2.21	0.70
1:A:528:ARG:HG3	1:A:529:LEU:CD2	2.22	0.70
1:A:734:LEU:HD22	1:A:738:LYS:NZ	2.06	0.69
1:A:404:GLY:HA2	1:A:407:HIS:HD2	1.57	0.69
1:A:227:LEU:HD22	1:A:230:ARG:HH22	1.56	0.69
1:A:528:ARG:HG2	1:A:529:LEU:HD23	1.75	0.69
1:A:653:ALA:HB3	1:A:658:VAL:HG23	1.73	0.69
1:A:614:THR:O	1:A:616:PRO:HD3	1.93	0.69
1:A:853:HIS:O	1:A:854:LEU:CG	2.41	0.68
1:A:504:ILE:HG12	1:A:555:LEU:HD13	1.74	0.68
1:A:149:GLU:CD	1:A:230:ARG:NH2	2.50	0.68
1:A:434:SER:O	1:A:438:ILE:HD13	1.92	0.68
1:A:608:LEU:HB3	1:A:629:ARG:HD3	1.75	0.68
1:A:756:ILE:HB	1:A:797:MET:CE	2.23	0.68
1:A:354:GLN:O	1:A:358:GLN:HG2	1.94	0.68
1:A:971:GLN:OE1	1:A:1049:ARG:NH2	2.24	0.68
1:A:558:LEU:HD23	1:A:559:ALA:N	2.08	0.68
1:A:131:VAL:O	1:A:135:ILE:HD13	1.93	0.68
1:A:797:MET:HG3	1:A:824:ILE:HD11	1.76	0.68
1:A:753:ALA:HA	1:A:756:ILE:CD1	2.23	0.68
1:A:205:LEU:O	1:A:209:MET:HG3	1.93	0.68
1:A:569:ALA:HA	1:A:572:ILE:HD11	1.76	0.68
1:A:9:ILE:HG22	1:A:9:ILE:O	1.94	0.67
1:A:318:ARG:HA	1:A:321:ILE:HD12	1.76	0.67
1:A:747:GLN:NE2	1:A:750:VAL:HG21	2.08	0.67
1:A:314:ALA:CB	1:A:317:GLU:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ILE:O	1:A:813:LEU:CD1	2.43	0.67
1:A:149:GLU:O	1:A:149:GLU:HG2	1.94	0.67
1:A:973:THR:HG21	1:A:1049:ARG:HG2	1.75	0.67
1:A:384:ILE:HD11	1:A:414:GLU:HB3	1.77	0.67
1:A:407:HIS:O	1:A:411:ILE:CG1	2.42	0.67
1:A:738:LYS:HA	1:A:741:MET:HG3	1.77	0.67
1:A:756:ILE:CG1	1:A:797:MET:CE	2.64	0.67
1:A:569:ALA:HA	1:A:572:ILE:CD1	2.25	0.67
1:A:525:GLU:HA	1:A:528:ARG:HD3	1.76	0.66
1:A:4:PHE:N	1:A:4:PHE:CD2	2.63	0.66
1:A:258:TRP:CZ2	1:A:486:PRO:HG3	2.30	0.66
1:A:533:MET:CE	1:A:537:TYR:CD2	2.79	0.65
1:A:730:ILE:HD11	1:A:759:ARG:HB3	1.78	0.65
1:A:9:ILE:HD12	1:A:123:LEU:HD22	1.79	0.65
1:A:141:ILE:HD13	1:A:171:MET:CE	2.27	0.65
1:A:853:HIS:CG	1:A:854:LEU:H	2.15	0.65
1:A:844:PRO:C	1:A:846:PRO:CD	2.69	0.65
1:A:427:GLU:O	1:A:431:ILE:HG12	1.97	0.64
1:A:514:VAL:HB	1:A:517:ALA:CB	2.26	0.64
1:A:255:GLU:O	1:A:258:TRP:HE3	1.78	0.64
1:A:504:ILE:CG2	1:A:505:ASP:N	2.60	0.64
1:A:976:ARG:CG	1:A:977:ILE:N	2.60	0.64
1:A:973:THR:CG2	1:A:1049:ARG:CG	2.69	0.64
1:A:1020:THR:O	1:A:1024:VAL:HG23	1.97	0.64
1:A:88:LEU:HD22	1:A:108:LEU:HD12	1.79	0.64
1:A:645:GLU:O	1:A:645:GLU:HG3	1.96	0.64
1:A:741:MET:HE1	1:A:817:PHE:CE2	2.32	0.64
1:A:756:ILE:HD12	1:A:797:MET:SD	2.38	0.64
1:A:503:TRP:HD1	1:A:515:GLY:HA3	1.63	0.64
1:A:404:GLY:HA2	1:A:407:HIS:CD2	2.33	0.64
1:A:504:ILE:CG2	1:A:505:ASP:H	2.11	0.64
1:A:583:LEU:O	1:A:587:MET:HG3	1.97	0.63
1:A:12:ILE:HD11	1:A:54:LEU:HD11	1.80	0.63
1:A:610:ALA:O	1:A:614:THR:CB	2.46	0.63
1:A:196:ASN:HA	1:A:199:LYS:CD	2.28	0.63
1:A:201:LEU:HD13	1:A:237:MET:HG2	1.80	0.63
1:A:881:LYS:O	1:A:882:ASP:HB2	1.98	0.63
1:A:220:SER:O	1:A:223:ILE:HG13	1.98	0.63
1:A:207:SER:O	1:A:694:HIS:HD2	1.81	0.62
1:A:1048:ILE:HD12	1:A:1048:ILE:H	1.65	0.62
1:A:614:THR:O	1:A:616:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:GLU:O	1:A:888:GLN:HB2	2.00	0.62
1:A:851:HIS:C	1:A:852:LEU:HD13	2.24	0.62
1:A:555:LEU:HG	1:A:572:ILE:HD12	1.81	0.62
1:A:3:VAL:HB	1:A:124:LEU:HD21	1.81	0.61
1:A:204:VAL:HG13	1:A:698:MET:HE1	1.83	0.61
1:A:605:PRO:HB2	1:A:633:PHE:CD1	2.36	0.61
1:A:895:ASN:C	1:A:897:PRO:HD3	2.25	0.61
1:A:273:ILE:HG23	1:A:302:ILE:HG23	1.82	0.61
1:A:853:HIS:O	1:A:854:LEU:CB	2.48	0.61
1:A:225:GLU:HB3	1:A:681:ILE:HD11	1.83	0.61
1:A:606:ILE:H	1:A:606:ILE:CD1	2.06	0.61
1:A:734:LEU:O	1:A:738:LYS:HG2	2.01	0.61
1:A:238:SER:HA	1:A:241:ILE:HD12	1.83	0.61
1:A:511:ASP:OD2	1:A:900:MET:SD	2.59	0.61
1:A:548:VAL:HG21	1:A:583:LEU:HD12	1.82	0.61
1:A:1011:ILE:O	1:A:1011:ILE:HG13	2.00	0.61
1:A:237:MET:O	1:A:241:ILE:HG13	2.00	0.60
1:A:492:HIS:O	1:A:496:LYS:HG3	2.01	0.60
1:A:645:GLU:O	1:A:646:LYS:C	2.44	0.60
1:A:504:ILE:HG13	1:A:576:LEU:HD21	1.83	0.60
1:A:509:VAL:HG12	1:A:510:ASP:N	2.15	0.60
1:A:23:LEU:HD21	1:A:40:LEU:HD11	1.84	0.60
1:A:314:ALA:C	1:A:485:ARG:HG2	2.27	0.60
1:A:291:PRO:O	1:A:296:GLU:HG3	2.01	0.60
1:A:4:PHE:HD2	1:A:4:PHE:N	2.00	0.60
1:A:650:VAL:HG12	1:A:650:VAL:O	2.02	0.60
1:A:225:GLU:CB	1:A:681:ILE:HD11	2.32	0.60
1:A:479:ARG:HG2	1:A:483:ASN:HB2	1.84	0.59
1:A:227:LEU:CD2	1:A:230:ARG:HH22	2.15	0.59
1:A:976:ARG:CG	1:A:977:ILE:H	2.15	0.59
1:A:422:CYS:SG	1:A:484:THR:HG21	2.43	0.59
1:A:74:MET:N	1:A:75:PRO:CD	2.66	0.59
1:A:610:ALA:O	1:A:614:THR:HB	2.02	0.59
1:A:947:LEU:HD23	1:A:947:LEU:O	2.02	0.59
1:A:15:PRO:O	1:A:19:GLN:HG2	2.02	0.59
1:A:24:VAL:CG1	1:A:948:ILE:HD11	2.33	0.59
1:A:513:GLY:O	1:A:514:VAL:HG13	2.02	0.59
1:A:653:ALA:HB3	1:A:658:VAL:CG2	2.33	0.59
1:A:258:TRP:CE2	1:A:486:PRO:HG3	2.38	0.58
1:A:408:ILE:O	1:A:412:MET:N	2.31	0.58
1:A:893:ALA:HB1	1:A:894:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD13	1:A:954:ILE:HG13	1.85	0.58
1:A:645:GLU:O	1:A:648:ALA:N	2.34	0.58
1:A:85:CYS:O	1:A:89:VAL:HG23	2.03	0.58
1:A:679:ALA:O	1:A:683:LEU:HB2	2.03	0.58
1:A:702:TRP:O	1:A:706:VAL:HG23	2.04	0.58
1:A:79:ILE:HG22	1:A:80:LYS:N	2.19	0.58
1:A:339:ARG:O	1:A:343:GLN:HA	2.04	0.58
1:A:893:ALA:C	1:A:894:ILE:HD12	2.29	0.58
1:A:741:MET:CE	1:A:817:PHE:HE2	2.01	0.57
1:A:532:VAL:O	1:A:532:VAL:HG12	2.04	0.57
1:A:613:ALA:HB2	1:A:683:LEU:CB	2.09	0.57
1:A:741:MET:HE3	1:A:817:PHE:CE2	2.38	0.57
1:A:153:THR:HG23	1:A:155:GLU:H	1.70	0.57
1:A:149:GLU:CG	1:A:230:ARG:NH1	2.55	0.56
1:A:528:ARG:CG	1:A:529:LEU:CD2	2.78	0.56
1:A:804:VAL:HA	1:A:813:LEU:HD22	1.87	0.56
1:A:397:ASP:N	1:A:398:PRO:HD3	2.21	0.56
1:A:930:MET:HA	1:A:930:MET:CE	2.26	0.56
1:A:68:GLN:OE1	1:A:71:LYS:HD2	2.05	0.56
1:A:529:LEU:N	1:A:529:LEU:CD2	2.64	0.56
1:A:606:ILE:HD13	1:A:606:ILE:N	2.13	0.56
1:A:734:LEU:HD21	1:A:756:ILE:HG21	1.88	0.56
1:A:73:ASP:C	1:A:76:PRO:HD2	2.31	0.56
1:A:23:LEU:HD22	1:A:108:LEU:HD11	1.87	0.56
1:A:69:ILE:HD13	1:A:69:ILE:N	2.18	0.56
1:A:621:ASN:O	1:A:622:ARG:C	2.48	0.56
1:A:752:GLY:O	1:A:756:ILE:CD1	2.46	0.56
1:A:795:SER:CB	1:A:796:PRO:HD3	2.34	0.56
1:A:809:SER:HB3	1:A:811:PRO:HD2	1.88	0.56
1:A:147:VAL:O	1:A:147:VAL:HG13	2.07	0.55
1:A:74:MET:HG2	1:A:125:THR:HG21	1.87	0.55
1:A:694:HIS:O	1:A:694:HIS:ND1	2.39	0.55
1:A:219:LYS:N	1:A:219:LYS:CD	2.70	0.55
1:A:310:GLY:O	1:A:313:CYS:HB2	2.06	0.55
1:A:572:ILE:HA	1:A:575:GLN:HG2	1.89	0.55
1:A:604:THR:HB	1:A:605:PRO:HD3	1.88	0.55
1:A:619:THR:H	1:A:620:PRO:CD	2.20	0.55
1:A:976:ARG:HG3	1:A:977:ILE:H	1.72	0.55
1:A:591:MET:CE	1:A:717:ILE:HD11	2.37	0.55
1:A:528:ARG:HH12	1:A:646:LYS:HZ2	1.53	0.54
1:A:603:THR:CA	1:A:606:ILE:HD11	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ALA:O	1:A:614:THR:OG1	2.23	0.54
1:A:500:ALA:HB2	1:A:518:ALA:HB3	1.88	0.54
1:A:601:ASP:O	1:A:603:THR:N	2.40	0.54
1:A:4:PHE:HD1	1:A:994:GLN:HG2	1.72	0.54
1:A:645:GLU:OE2	1:A:649:ALA:HB2	2.08	0.54
1:A:1057:ARG:HD3	1:A:1059:VAL:HG23	1.89	0.54
1:A:81:VAL:HG13	1:A:82:GLU:N	2.23	0.54
1:A:171:MET:O	1:A:175:ILE:HG12	2.06	0.54
1:A:614:THR:C	1:A:616:PRO:HD3	2.32	0.54
1:A:503:TRP:HH2	1:A:511:ASP:HB3	1.71	0.54
1:A:74:MET:HE3	1:A:122:LEU:HD12	1.90	0.54
1:A:153:THR:HG22	1:A:156:ASP:H	1.72	0.54
1:A:1062:THR:C	1:A:1064:TRP:H	2.16	0.53
1:A:27:HIS:ND1	1:A:108:LEU:HD23	2.23	0.53
1:A:219:LYS:CD	1:A:219:LYS:H	2.20	0.53
1:A:509:VAL:O	1:A:510:ASP:HB2	2.07	0.53
1:A:1045:SER:C	1:A:1048:ILE:HD11	2.28	0.53
1:A:273:ILE:HG23	1:A:302:ILE:HD12	1.89	0.53
1:A:207:SER:O	1:A:694:HIS:CD2	2.61	0.53
1:A:324:THR:O	1:A:324:THR:HG22	2.08	0.53
1:A:233:THR:O	1:A:237:MET:HG3	2.08	0.53
1:A:682:LEU:O	1:A:683:LEU:HG	2.08	0.53
1:A:729:ALA:HB3	1:A:759:ARG:NH2	2.23	0.53
1:A:738:LYS:HD2	1:A:817:PHE:CZ	2.43	0.53
1:A:894:ILE:HG22	1:A:895:ASN:N	2.22	0.53
1:A:591:MET:SD	1:A:717:ILE:CG1	2.92	0.53
1:A:3:VAL:HG13	1:A:251:THR:HG23	1.90	0.53
1:A:5:HIS:CD2	1:A:6:THR:HG22	2.44	0.53
1:A:9:ILE:HG23	1:A:123:LEU:HD13	1.90	0.53
1:A:504:ILE:CD1	1:A:576:LEU:HD23	2.40	0.52
1:A:808:ILE:O	1:A:813:LEU:CG	2.54	0.52
1:A:67:ASP:CB	1:A:70:LEU:HD22	2.39	0.52
1:A:1023:LEU:O	1:A:1023:LEU:HG	2.09	0.52
1:A:37:ILE:HG21	1:A:95:LEU:HD13	1.92	0.52
1:A:292:GLY:HA2	1:A:296:GLU:HB2	1.90	0.52
1:A:735:ASP:HA	1:A:738:LYS:HG2	1.91	0.52
1:A:804:VAL:HG22	1:A:813:LEU:HD22	1.91	0.52
1:A:1:MET:HE1	1:A:1022:MET:HE3	1.91	0.52
1:A:665:VAL:HG22	1:A:709:MET:HE2	1.91	0.52
1:A:398:PRO:O	1:A:400:GLY:N	2.42	0.52
1:A:503:TRP:HH2	1:A:511:ASP:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG23	1:A:33:ASP:OD1	2.10	0.51
1:A:804:VAL:HG12	1:A:804:VAL:O	2.10	0.51
1:A:920:ILE:HD11	1:A:1058:TRP:CZ3	2.46	0.51
1:A:1054:PHE:CD1	1:A:1054:PHE:C	2.88	0.51
1:A:854:LEU:O	1:A:855:THR:O	2.29	0.51
1:A:896:GLN:N	1:A:897:PRO:CD	2.73	0.51
1:A:756:ILE:CD1	1:A:797:MET:SD	2.99	0.51
1:A:729:ALA:CB	1:A:759:ARG:HH22	2.22	0.51
1:A:504:ILE:C	1:A:504:ILE:HD13	2.36	0.51
1:A:74:MET:HE2	1:A:122:LEU:HD12	1.84	0.51
1:A:245:ILE:HA	1:A:248:LEU:HD12	1.93	0.51
1:A:-2:VAL:C	1:A:-1:PRO:CA	2.70	0.50
1:A:13:LEU:O	1:A:16:VAL:HG12	2.11	0.50
1:A:69:ILE:H	1:A:69:ILE:CD1	2.13	0.50
1:A:258:TRP:CZ2	1:A:486:PRO:CG	2.94	0.50
1:A:551:LEU:HD13	1:A:575:GLN:HG3	1.94	0.50
1:A:595:VAL:HG12	1:A:595:VAL:O	2.11	0.50
1:A:493:LEU:O	1:A:497:ILE:HG12	2.12	0.50
1:A:703:ILE:CD1	1:A:703:ILE:N	2.75	0.50
1:A:1049:ARG:O	1:A:1052:ALA:N	2.43	0.50
1:A:391:ALA:HA	1:A:407:HIS:CG	2.46	0.50
1:A:222:GLY:HA3	1:A:681:ILE:HG12	1.93	0.50
1:A:887:GLU:HG2	1:A:903:ARG:NH2	2.26	0.50
1:A:538:ARG:HG3	1:A:542:LEU:HD12	1.94	0.49
1:A:636:HIS:O	1:A:640:LEU:HG	2.12	0.49
1:A:754:THR:O	1:A:757:ALA:HB3	2.12	0.49
1:A:793:THR:CG2	1:A:824:ILE:HG12	2.42	0.49
1:A:808:ILE:H	1:A:813:LEU:HD11	1.73	0.49
1:A:94:MET:SD	1:A:104:ALA:HB2	2.52	0.49
1:A:134:ILE:HG13	1:A:174:MET:HE2	1.93	0.49
1:A:391:ALA:HB2	1:A:407:HIS:CG	2.47	0.49
1:A:553:ALA:C	1:A:555:LEU:H	2.20	0.49
1:A:646:LYS:O	1:A:650:VAL:HG23	2.11	0.49
1:A:74:MET:CG	1:A:125:THR:HG21	2.41	0.49
1:A:135:ILE:CD1	1:A:135:ILE:N	2.75	0.49
1:A:694:HIS:ND1	1:A:694:HIS:C	2.70	0.49
1:A:9:ILE:O	1:A:9:ILE:CG2	2.60	0.49
1:A:754:THR:HG22	1:A:758:ARG:HE	1.77	0.49
1:A:764:LEU:HD21	1:A:790:LEU:HB2	1.95	0.49
1:A:1062:THR:HG22	1:A:1063:PRO:HD3	1.95	0.49
1:A:7:ARG:HB3	1:A:181:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:THR:N	1:A:620:PRO:CD	2.76	0.49
1:A:760:ALA:CB	1:A:794:ILE:HD11	2.43	0.49
1:A:14:GLU:N	1:A:15:PRO:HD2	2.28	0.48
1:A:205:LEU:O	1:A:209:MET:CG	2.59	0.48
1:A:215:THR:HG21	1:A:223:ILE:HA	1.94	0.48
1:A:793:THR:HG21	1:A:824:ILE:HA	1.94	0.48
1:A:403:GLU:C	1:A:405:GLU:H	2.21	0.48
1:A:558:LEU:O	1:A:561:ARG:HG2	2.12	0.48
1:A:94:MET:HG2	1:A:95:LEU:N	2.28	0.48
1:A:134:ILE:N	1:A:134:ILE:HD12	2.29	0.48
1:A:658:VAL:O	1:A:662:GLN:HG3	2.13	0.48
1:A:930:MET:CE	1:A:933:MET:SD	2.98	0.48
1:A:24:VAL:HG12	1:A:948:ILE:HD11	1.95	0.48
1:A:75:PRO:N	1:A:76:PRO:CD	2.75	0.48
1:A:287:PRO:HB3	1:A:345:ALA:HB2	1.95	0.48
1:A:408:ILE:CG2	1:A:412:MET:SD	2.99	0.48
1:A:741:MET:SD	1:A:817:PHE:CZ	3.05	0.48
1:A:656:THR:O	1:A:656:THR:CG2	2.60	0.48
1:A:886:PRO:HB2	1:A:889:LYS:HE2	1.95	0.48
1:A:25:ILE:HG23	1:A:948:ILE:HD13	1.95	0.48
1:A:310:GLY:HA2	1:A:321:ILE:HD13	1.95	0.48
1:A:445:LEU:HD11	1:A:466:ILE:HD12	1.95	0.48
1:A:981:LEU:O	1:A:984:VAL:HG12	2.14	0.48
1:A:0:ARG:O	1:A:1:MET:SD	2.72	0.47
1:A:3:VAL:C	1:A:4:PHE:CD2	2.87	0.47
1:A:288:ASN:O	1:A:290:PRO:HD3	2.14	0.47
1:A:755:SER:O	1:A:756:ILE:C	2.56	0.47
1:A:609:LEU:HD21	1:A:633:PHE:HB2	1.96	0.47
1:A:234:VAL:O	1:A:234:VAL:HG12	2.14	0.47
1:A:661:ILE:O	1:A:664:THR:HB	2.14	0.47
1:A:920:ILE:HD11	1:A:1058:TRP:CH2	2.49	0.47
1:A:930:MET:SD	1:A:1031:MET:HE3	2.54	0.47
1:A:408:ILE:HD12	1:A:408:ILE:N	2.30	0.47
1:A:808:ILE:H	1:A:813:LEU:HD21	1.79	0.47
1:A:67:ASP:OD2	1:A:69:ILE:HD11	2.15	0.47
1:A:660:GLY:O	1:A:661:ILE:C	2.58	0.47
1:A:710:THR:HG23	1:A:762:ARG:NH2	2.30	0.47
1:A:919:ILE:HD11	1:A:964:LEU:HB3	1.97	0.47
1:A:74:MET:CE	1:A:74:MET:CG	2.91	0.47
1:A:509:VAL:HG12	1:A:510:ASP:H	1.80	0.47
1:A:804:VAL:HG13	1:A:813:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:GLU:O	1:A:840:PRO:C	2.57	0.47
1:A:843:PRO:C	1:A:845:PRO:HD2	2.40	0.47
1:A:919:ILE:HG13	1:A:964:LEU:HD13	1.97	0.47
1:A:853:HIS:C	1:A:854:LEU:HG	2.40	0.47
1:A:346:THR:HB	1:A:347:PRO:HD2	1.96	0.46
1:A:498:GLU:OE1	1:A:1035:LYS:NZ	2.43	0.46
1:A:141:ILE:CD1	1:A:171:MET:SD	3.01	0.46
1:A:258:TRP:CG	1:A:259:ALA:N	2.83	0.46
1:A:555:LEU:CG	1:A:572:ILE:HD12	2.44	0.46
1:A:572:ILE:O	1:A:576:LEU:HB3	2.15	0.46
1:A:746:PRO:O	1:A:747:GLN:HB2	2.14	0.46
1:A:314:ALA:HB1	1:A:485:ARG:NE	2.30	0.46
1:A:313:CYS:SG	1:A:321:ILE:HD13	2.56	0.46
1:A:773:ASN:CG	1:A:773:ASN:O	2.58	0.46
1:A:882:ASP:OD2	1:A:1061:LYS:NZ	2.46	0.46
1:A:1064:TRP:HA	1:A:1064:TRP:CE3	2.51	0.46
1:A:9:ILE:CD1	1:A:123:LEU:HB3	2.40	0.46
1:A:504:ILE:HG12	1:A:555:LEU:CD1	2.43	0.46
1:A:555:LEU:HD21	1:A:572:ILE:CD1	2.46	0.46
1:A:619:THR:H	1:A:620:PRO:HD3	1.78	0.46
1:A:623:GLU:O	1:A:624:GLU:C	2.57	0.46
1:A:391:ALA:CB	1:A:407:HIS:CG	2.98	0.46
1:A:548:VAL:HG21	1:A:583:LEU:CD1	2.46	0.46
1:A:734:LEU:HB3	1:A:738:LYS:CE	2.41	0.46
1:A:853:HIS:CG	1:A:854:LEU:N	2.83	0.46
1:A:484:THR:OG1	1:A:485:ARG:N	2.49	0.46
1:A:609:LEU:HD11	1:A:633:PHE:CG	2.52	0.46
1:A:613:ALA:HB2	1:A:683:LEU:CD1	2.29	0.46
1:A:974:ASP:O	1:A:975:LYS:C	2.58	0.46
1:A:134:ILE:HD12	1:A:134:ILE:H	1.80	0.45
1:A:220:SER:O	1:A:222:GLY:N	2.49	0.45
1:A:258:TRP:CD1	1:A:258:TRP:C	2.93	0.45
1:A:300:ARG:HB3	1:A:531:ASN:HD21	1.80	0.45
1:A:470:LEU:O	1:A:470:LEU:HD23	2.17	0.45
1:A:502:ARG:HD3	1:A:502:ARG:N	2.31	0.45
1:A:756:ILE:CD1	1:A:797:MET:HE1	2.42	0.45
1:A:894:ILE:HD12	1:A:894:ILE:N	2.32	0.45
1:A:1012:SER:HB2	1:A:1015:GLU:HB2	1.98	0.45
1:A:1048:ILE:HG22	1:A:1052:ALA:CB	2.46	0.45
1:A:555:LEU:HD21	1:A:572:ILE:HD11	1.98	0.45
1:A:820:SER:O	1:A:824:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:GLU:HG3	1:A:880:GLU:HG3	1.99	0.45
1:A:133:LYS:HZ3	1:A:174:MET:HE3	1.81	0.45
1:A:215:THR:O	1:A:215:THR:HG22	2.15	0.45
1:A:653:ALA:O	1:A:657:THR:CB	2.52	0.45
1:A:67:ASP:HB3	1:A:70:LEU:HD22	1.97	0.45
1:A:574:ALA:O	1:A:578:ASP:OD2	2.33	0.45
1:A:889:LYS:HD3	1:A:935:ARG:NH1	2.32	0.45
1:A:23:LEU:CD2	1:A:40:LEU:HD11	2.47	0.45
1:A:396:ALA:O	1:A:397:ASP:HB2	2.17	0.45
1:A:397:ASP:N	1:A:397:ASP:OD1	2.50	0.45
1:A:591:MET:HE1	1:A:717:ILE:HD11	1.99	0.45
1:A:682:LEU:O	1:A:683:LEU:CG	2.64	0.45
1:A:797:MET:HE2	1:A:824:ILE:HD13	1.99	0.45
1:A:997:ILE:N	1:A:997:ILE:HD12	2.32	0.44
1:A:356:VAL:O	1:A:360:LEU:HG	2.16	0.44
1:A:14:GLU:HG2	1:A:993:THR:HG21	1.99	0.44
1:A:74:MET:N	1:A:75:PRO:HD2	2.32	0.44
1:A:234:VAL:O	1:A:234:VAL:CG1	2.66	0.44
1:A:853:HIS:O	1:A:854:LEU:HB2	2.17	0.44
1:A:70:LEU:HD11	1:A:129:ALA:HB2	1.99	0.44
1:A:273:ILE:HA	1:A:302:ILE:CD1	2.48	0.44
1:A:408:ILE:O	1:A:412:MET:CG	2.62	0.44
1:A:877:PRO:N	1:A:878:PRO:HD2	2.33	0.44
1:A:441:LEU:O	1:A:466:ILE:HD11	2.16	0.44
1:A:504:ILE:CG1	1:A:576:LEU:CD2	2.78	0.44
1:A:739:VAL:C	1:A:741:MET:H	2.25	0.44
1:A:790:LEU:O	1:A:794:ILE:HG12	2.17	0.44
1:A:12:ILE:CD1	1:A:54:LEU:HD11	2.45	0.44
1:A:211:ILE:HD11	1:A:694:HIS:CB	2.48	0.44
1:A:470:LEU:HD23	1:A:470:LEU:C	2.43	0.44
1:A:755:SER:C	1:A:757:ALA:N	2.75	0.44
1:A:844:PRO:HA	1:A:846:PRO:HD2	1.99	0.44
1:A:285:ARG:O	1:A:287:PRO:HD2	2.13	0.44
1:A:314:ALA:CB	1:A:485:ARG:HD3	2.47	0.44
1:A:314:ALA:HB1	1:A:485:ARG:CZ	2.48	0.44
1:A:703:ILE:O	1:A:703:ILE:HG22	2.17	0.44
1:A:219:LYS:HB2	1:A:223:ILE:HD11	2.00	0.44
1:A:940:GLY:HA2	1:A:943:ASN:HB2	2.00	0.44
1:A:665:VAL:HG22	1:A:709:MET:CE	2.48	0.43
1:A:821:GLY:HA2	1:A:824:ILE:HD12	2.00	0.43
1:A:854:LEU:O	1:A:855:THR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:ASP:HB3	1:A:977:ILE:HG22	2.00	0.43
1:A:509:VAL:CG1	1:A:510:ASP:N	2.81	0.43
1:A:843:PRO:N	1:A:844:PRO:HD2	2.33	0.43
1:A:848:ASP:O	1:A:850:GLU:HG3	2.18	0.43
1:A:971:GLN:CG	1:A:1053:GLY:H	2.32	0.43
1:A:100:TYR:CD1	1:A:100:TYR:N	2.85	0.43
1:A:619:THR:HB	1:A:620:PRO:HD3	2.00	0.43
1:A:793:THR:HG22	1:A:824:ILE:HG12	2.00	0.43
1:A:1048:ILE:HG22	1:A:1052:ALA:HB2	2.00	0.43
1:A:644:ALA:O	1:A:645:GLU:C	2.60	0.43
1:A:741:MET:HE1	1:A:814:GLN:HA	1.99	0.43
1:A:880:GLU:O	1:A:881:LYS:HB3	2.18	0.43
1:A:747:GLN:NE2	1:A:750:VAL:CG2	2.80	0.43
1:A:664:THR:CG2	1:A:709:MET:HG3	2.49	0.43
1:A:178:ARG:HA	1:A:178:ARG:HD2	1.87	0.43
1:A:643:THR:O	1:A:643:THR:HG22	2.18	0.43
1:A:804:VAL:O	1:A:805:ALA:C	2.61	0.43
1:A:887:GLU:O	1:A:888:GLN:CB	2.65	0.43
1:A:1037:THR:O	1:A:1037:THR:HG22	2.19	0.43
1:A:412:MET:HE3	1:A:438:ILE:HG22	2.00	0.43
1:A:807:ASN:C	1:A:813:LEU:HD11	2.43	0.43
1:A:917:ASN:OD1	1:A:920:ILE:HG12	2.19	0.43
1:A:195:MET:O	1:A:199:LYS:HG3	2.19	0.42
1:A:844:PRO:CA	1:A:846:PRO:HD2	2.48	0.42
1:A:24:VAL:HG11	1:A:948:ILE:HD11	2.01	0.42
1:A:1062:THR:HB	1:A:1063:PRO:CD	2.49	0.42
1:A:34:GLY:O	1:A:36:ALA:N	2.52	0.42
1:A:645:GLU:O	1:A:648:ALA:HB3	2.19	0.42
1:A:982:LEU:O	1:A:986:GLU:HB2	2.20	0.42
1:A:215:THR:CG2	1:A:223:ILE:HG12	2.49	0.42
1:A:81:VAL:CG1	1:A:82:GLU:N	2.83	0.42
1:A:102:VAL:O	1:A:105:ARG:HG2	2.20	0.42
1:A:219:LYS:N	1:A:219:LYS:HD2	2.35	0.42
1:A:642:ALA:O	1:A:646:LYS:HG2	2.19	0.42
1:A:947:LEU:HD23	1:A:947:LEU:C	2.44	0.42
1:A:967:GLU:HB3	1:A:1054:PHE:CE2	2.55	0.42
1:A:9:ILE:HD12	1:A:123:LEU:CB	2.46	0.42
1:A:738:LYS:HD2	1:A:817:PHE:HZ	1.85	0.42
1:A:929:LEU:HB3	1:A:954:ILE:HD11	2.00	0.42
1:A:149:GLU:CB	1:A:230:ARG:CZ	2.97	0.42
1:A:894:ILE:CG2	1:A:895:ASN:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:MET:HE3	1:A:94:MET:HB3	1.90	0.42
1:A:194:SER:HB2	1:A:244:ILE:HD11	2.01	0.42
1:A:266:MET:HE3	1:A:266:MET:HB3	1.95	0.42
1:A:503:TRP:CH2	1:A:511:ASP:HB3	2.53	0.42
1:A:631:ALA:O	1:A:635:ASN:ND2	2.53	0.42
1:A:682:LEU:O	1:A:683:LEU:HD23	2.20	0.42
1:A:1048:ILE:HD12	1:A:1048:ILE:N	2.32	0.42
1:A:405:GLU:O	1:A:409:ARG:HB2	2.20	0.42
1:A:501:GLN:HA	1:A:504:ILE:HG22	2.02	0.42
1:A:558:LEU:HD23	1:A:559:ALA:HB2	2.02	0.42
1:A:702:TRP:CE3	1:A:703:ILE:HD12	2.44	0.42
1:A:522:LEU:HD13	1:A:580:LEU:HD22	2.02	0.41
1:A:653:ALA:HB1	1:A:657:THR:HB	2.02	0.41
1:A:703:ILE:O	1:A:707:GLU:HG3	2.20	0.41
1:A:703:ILE:HG22	1:A:707:GLU:HG3	2.02	0.41
1:A:876:PRO:HA	1:A:877:PRO:HD3	1.62	0.41
1:A:930:MET:HE3	1:A:933:MET:HB3	2.01	0.41
1:A:973:THR:O	1:A:973:THR:OG1	2.25	0.41
1:A:91:ALA:HA	1:A:94:MET:SD	2.60	0.41
1:A:396:ALA:O	1:A:397:ASP:CB	2.68	0.41
1:A:845:PRO:O	1:A:847:PRO:HD2	2.06	0.41
1:A:852:LEU:HD12	1:A:852:LEU:HA	1.67	0.41
1:A:853:HIS:CE1	1:A:855:THR:OG1	2.72	0.41
1:A:930:MET:CE	1:A:933:MET:HB3	2.50	0.41
1:A:149:GLU:HB2	1:A:230:ARG:NE	2.35	0.41
1:A:363:LEU:C	1:A:363:LEU:HD23	2.45	0.41
1:A:938:ARG:HA	1:A:938:ARG:HD3	1.92	0.41
1:A:714:ASP:C	1:A:716:ALA:H	2.28	0.41
1:A:722:LEU:HD23	1:A:722:LEU:C	2.45	0.41
1:A:314:ALA:H	1:A:318:ARG:HB2	1.86	0.41
1:A:604:THR:N	1:A:605:PRO:CD	2.83	0.41
1:A:227:LEU:HD22	1:A:230:ARG:NH2	2.29	0.41
1:A:758:ARG:H	1:A:758:ARG:HG3	1.57	0.41
1:A:672:THR:N	1:A:673:PRO:CD	2.84	0.41
1:A:771:VAL:HG13	1:A:780:ARG:HG3	2.01	0.41
1:A:1049:ARG:O	1:A:1051:ASP:N	2.53	0.41
1:A:42:ALA:N	1:A:43:PRO:HD2	2.35	0.41
1:A:211:ILE:HD11	1:A:694:HIS:CG	2.56	0.41
1:A:377:MET:HB3	1:A:481:VAL:CG1	2.51	0.41
1:A:719:THR:O	1:A:720:LYS:C	2.64	0.41
1:A:755:SER:O	1:A:759:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ILE:HD11	1:A:1000:THR:HG22	2.03	0.41
1:A:188:ARG:O	1:A:192:VAL:HG23	2.21	0.41
1:A:100:TYR:O	1:A:101:SER:C	2.64	0.40
1:A:399:ASN:HD22	1:A:399:ASN:HA	1.71	0.40
1:A:194:SER:CB	1:A:244:ILE:HD11	2.51	0.40
1:A:540:ASP:O	1:A:544:LYS:HG2	2.21	0.40
1:A:16:VAL:CG1	1:A:17:ALA:N	2.83	0.40
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.78	0.40
1:A:98:ASP:C	1:A:100:TYR:H	2.28	0.40
1:A:572:ILE:O	1:A:576:LEU:CB	2.70	0.40
1:A:760:ALA:HB1	1:A:794:ILE:HD11	2.04	0.40
1:A:988:ILE:N	1:A:989:PRO:CD	2.84	0.40
1:A:442:THR:O	1:A:442:THR:HG22	2.20	0.40
1:A:775:GLU:O	1:A:776:ASP:C	2.63	0.40
1:A:25:ILE:HG23	1:A:948:ILE:CD1	2.50	0.40
1:A:65:THR:HG21	1:A:70:LEU:HD23	2.04	0.40
1:A:495:GLY:O	1:A:498:GLU:HG2	2.22	0.40
1:A:506:ASN:O	1:A:508:THR:N	2.54	0.40
1:A:1045:SER:O	1:A:1045:SER:OG	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MET:CE	1:A:743:ASN:CB[3_655]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1045/1069 (98%)	898 (86%)	93 (9%)	54 (5%)	1 10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	PRO
1	A	221	GLN
1	A	290	PRO
1	A	291	PRO
1	A	397	ASP
1	A	399	ASN
1	A	453	LYS
1	A	489	ALA
1	A	510	ASP
1	A	535	GLY
1	A	565	GLU
1	A	743	ASN
1	A	809	SER
1	A	810	ASP
1	A	850	GLU
1	A	882	ASP
1	A	1050	THR
1	A	426	LYS
1	A	837	PRO
1	A	841	ASP
1	A	854	LEU
1	A	881	LYS
1	A	895	ASN
1	A	1011	ILE
1	A	101	SER
1	A	288	ASN
1	A	394	TRP
1	A	400	GLY
1	A	602	THR
1	A	615	ALA
1	A	622	ARG
1	A	846	PRO
1	A	878	PRO
1	A	879	GLU
1	A	888	GLN
1	A	975	LYS
1	A	33	ASP
1	A	39	ASP
1	A	287	PRO
1	A	558	LEU
1	A	616	PRO
1	A	624	GLU

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Mol	Chain	Res	Type
1	A	1062	THR
1	A	295	GLY
1	A	654	ASN
1	A	842	PHE
1	A	745	GLN
1	A	746	PRO
1	A	805	ALA
1	A	877	PRO
1	A	38	PRO
1	A	485	ARG
1	A	620	PRO
1	A	840	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	861/879 (98%)	735 (85%)	126 (15%)	3 14

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	4	PHE
1	A	6	THR
1	A	7	ARG
1	A	57	VAL
1	A	64	THR
1	A	65	THR
1	A	67	ASP
1	A	68	GLN
1	A	69	ILE
1	A	70	LEU
1	A	74	MET
1	A	79	ILE
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	94	MET
1	A	96	GLN
1	A	102	VAL
1	A	135	ILE
1	A	146	THR
1	A	147	VAL
1	A	150	VAL
1	A	152	GLU
1	A	153	THR
1	A	154	MET
1	A	156	ASP
1	A	177	GLU
1	A	199	LYS
1	A	207	SER
1	A	209	MET
1	A	211	ILE
1	A	218	THR
1	A	219	LYS
1	A	221	GLN
1	A	224	GLU
1	A	237	MET
1	A	246	ARG
1	A	253	TRP
1	A	254	ASP
1	A	256	ASP
1	A	258	TRP
1	A	268	ARG
1	A	270	LEU
1	A	272	LEU
1	A	287	PRO
1	A	290	PRO
1	A	291	PRO
1	A	313	CYS
1	A	316	LYS
1	A	341	ARG
1	A	364	THR
1	A	397	ASP
1	A	399	ASN
1	A	403	GLU
1	A	414	GLU
1	A	424	GLU
1	A	430	ASP

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Mol	Chain	Res	Type
1	A	481	VAL
1	A	486	PRO
1	A	488	LYS
1	A	499	GLN
1	A	501	GLN
1	A	502	ARG
1	A	504	ILE
1	A	505	ASP
1	A	514	VAL
1	A	528	ARG
1	A	529	LEU
1	A	534	MET
1	A	541	LEU
1	A	550	GLN
1	A	565	GLU
1	A	572	ILE
1	A	583	LEU
1	A	586	ARG
1	A	594	GLU
1	A	602	THR
1	A	606	ILE
1	A	619	THR
1	A	624	GLU
1	A	626	PHE
1	A	645	GLU
1	A	655	LYS
1	A	685	ASN
1	A	699	LYS
1	A	703	ILE
1	A	709	MET
1	A	741	MET
1	A	743	ASN
1	A	746	PRO
1	A	748	MET
1	A	756	ILE
1	A	770	GLU
1	A	807	ASN
1	A	808	ILE
1	A	810	ASP
1	A	817	PHE
1	A	832	ARG
1	A	836	GLN

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Mol	Chain	Res	Type
1	A	840	PRO
1	A	843	PRO
1	A	844	PRO
1	A	845	PRO
1	A	846	PRO
1	A	847	PRO
1	A	848	ASP
1	A	849	LEU
1	A	850	GLU
1	A	852	LEU
1	A	855	THR
1	A	875	PRO
1	A	876	PRO
1	A	882	ASP
1	A	904	GLN
1	A	944	LYS
1	A	971	GLN
1	A	972	CYS
1	A	1006	LEU
1	A	1008	ARG
1	A	1009	THR
1	A	1013	ASP
1	A	1045	SER
1	A	1048	ILE
1	A	1049	ARG
1	A	1057	ARG
1	A	1062	THR
1	A	1065	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	63	GLN
1	A	83	ASN
1	A	184	HIS
1	A	185	GLN
1	A	221	GLN
1	A	229	ASN
1	A	297	GLN
1	A	399	ASN
1	A	407	HIS

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Mol	Chain	Res	Type
1	A	465	GLN
1	A	472	ASN
1	A	474	GLN
1	A	478	ASN
1	A	554	GLN
1	A	575	GLN
1	A	577	GLN
1	A	635	ASN
1	A	674	GLN
1	A	694	HIS
1	A	700	ASN
1	A	701	GLN
1	A	747	GLN
1	A	814	GLN
1	A	980	ASN
1	A	1010	ASN
1	A	1026	ASN
1	A	1028	GLN
1	A	1029	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 oligosaccharides 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(Å ²)	Q<0.9
1	A	1049/1069 (98%)	0.33	30 (2%) 53 32	31, 125, 181, 205	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	THR	4.0
1	A	23	LEU	3.8
1	A	888	GLN	3.7
1	A	510	ASP	3.2
1	A	1055	THR	3.2
1	A	164	LEU	3.1
1	A	717	ILE	2.8
1	A	344	GLY	2.7
1	A	738	LYS	2.7
1	A	116	LEU	2.6
1	A	695	PHE	2.6
1	A	895	ASN	2.6
1	A	609	LEU	2.6
1	A	54	LEU	2.6
1	A	653	ALA	2.5
1	A	389	ASP	2.4
1	A	4	PHE	2.4
1	A	241	ILE	2.3
1	A	395	LEU	2.3
1	A	112	SER	2.3
1	A	88	LEU	2.2
1	A	525	GLU	2.2
1	A	150	VAL	2.2
1	A	749	LEU	2.1
1	A	118	GLY	2.1
1	A	9	ILE	2.1
1	A	734	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	522	LEU	2.1
1	A	750	VAL	2.0
1	A	879	GLU	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.