Full wwPDB EM Validation Report ⓘ

Feb 6, 2024 – 08:36 PM JST

PDB ID	:	8IVQ
EMDB ID	:	EMD-35759
Title	:	Cryo-EM structure of mouse BIRC6, Global map
Authors	:	Liu, S.; Jiang, T.; Bu, F.; Zhao, J.; Wang, G.; Li, N.; Gao, N.; Qiu, X.
Deposited on	:	2023-03-28
Resolution	:	3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

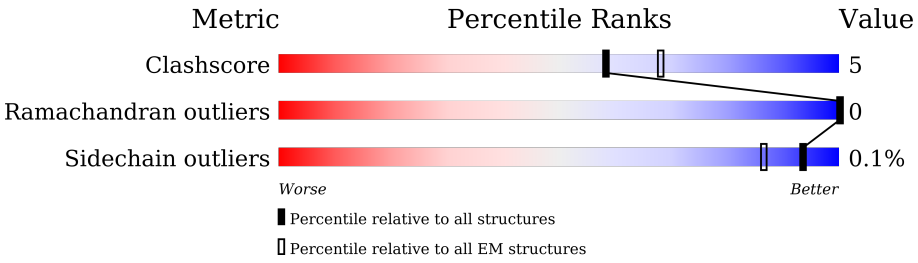
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	4896	52% 7% 40%
1	B	4896	52% 7% 40%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 41900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Isoform 2 of Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2921	Total	C	N	O	S	0	0
			20950	13236	3680	3904	130		
1	B	2921	Total	C	N	O	S	0	0
			20950	13236	3680	3904	130		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	MET	-	initiating methionine	UNP O88738
A	-49	ASP	-	expression tag	UNP O88738
A	-48	TYR	-	expression tag	UNP O88738
A	-47	LYS	-	expression tag	UNP O88738
A	-46	ASP	-	expression tag	UNP O88738
A	-45	HIS	-	expression tag	UNP O88738
A	-44	ASP	-	expression tag	UNP O88738
A	-43	GLY	-	expression tag	UNP O88738
A	-42	ASP	-	expression tag	UNP O88738
A	-41	TYR	-	expression tag	UNP O88738
A	-40	LYS	-	expression tag	UNP O88738
A	-39	ASP	-	expression tag	UNP O88738
A	-38	HIS	-	expression tag	UNP O88738
A	-37	ASP	-	expression tag	UNP O88738
A	-36	ILE	-	expression tag	UNP O88738
A	-35	ASP	-	expression tag	UNP O88738
A	-34	TYR	-	expression tag	UNP O88738
A	-33	LYS	-	expression tag	UNP O88738
A	-32	ASP	-	expression tag	UNP O88738
A	-31	ASP	-	expression tag	UNP O88738
A	-30	ASP	-	expression tag	UNP O88738
A	-29	ASP	-	expression tag	UNP O88738
A	-28	LYS	-	expression tag	UNP O88738
A	-27	ARG	-	expression tag	UNP O88738
A	-26	VAL	-	expression tag	UNP O88738
A	-25	VAL	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	PRO	-	expression tag	UNP O88738
A	-23	LEU	-	expression tag	UNP O88738
A	-22	GLU	-	expression tag	UNP O88738
A	-21	SER	-	expression tag	UNP O88738
A	-20	THR	-	expression tag	UNP O88738
A	-19	GLY	-	expression tag	UNP O88738
A	-18	LEU	-	expression tag	UNP O88738
A	-17	GLN	-	expression tag	UNP O88738
A	-16	GLU	-	expression tag	UNP O88738
A	-15	LEU	-	expression tag	UNP O88738
A	-14	ALA	-	expression tag	UNP O88738
A	-13	THR	-	expression tag	UNP O88738
A	-12	MET	-	expression tag	UNP O88738
A	-11	GLU	-	expression tag	UNP O88738
A	-10	GLN	-	expression tag	UNP O88738
A	-9	LYS	-	expression tag	UNP O88738
A	-8	LEU	-	expression tag	UNP O88738
A	-7	ILE	-	expression tag	UNP O88738
A	-6	SER	-	expression tag	UNP O88738
A	-5	GLU	-	expression tag	UNP O88738
A	-4	GLU	-	expression tag	UNP O88738
A	-3	ASP	-	expression tag	UNP O88738
A	-2	LEU	-	expression tag	UNP O88738
A	-1	GLU	-	expression tag	UNP O88738
A	0	PHE	-	expression tag	UNP O88738
A	178	ILE	THR	conflict	UNP O88738
A	690	THR	ALA	conflict	UNP O88738
A	2079	ARG	GLY	conflict	UNP O88738
A	2418	GLY	CYS	conflict	UNP O88738
A	2959	ILE	THR	conflict	UNP O88738
A	3226	THR	SER	conflict	UNP O88738
A	3914	VAL	MET	conflict	UNP O88738
A	3929	VAL	ILE	conflict	UNP O88738
A	4346	MET	VAL	conflict	UNP O88738
B	-50	MET	-	initiating methionine	UNP O88738
B	-49	ASP	-	expression tag	UNP O88738
B	-48	TYR	-	expression tag	UNP O88738
B	-47	LYS	-	expression tag	UNP O88738
B	-46	ASP	-	expression tag	UNP O88738
B	-45	HIS	-	expression tag	UNP O88738
B	-44	ASP	-	expression tag	UNP O88738
B	-43	GLY	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	ASP	-	expression tag	UNP O88738
B	-41	TYR	-	expression tag	UNP O88738
B	-40	LYS	-	expression tag	UNP O88738
B	-39	ASP	-	expression tag	UNP O88738
B	-38	HIS	-	expression tag	UNP O88738
B	-37	ASP	-	expression tag	UNP O88738
B	-36	ILE	-	expression tag	UNP O88738
B	-35	ASP	-	expression tag	UNP O88738
B	-34	TYR	-	expression tag	UNP O88738
B	-33	LYS	-	expression tag	UNP O88738
B	-32	ASP	-	expression tag	UNP O88738
B	-31	ASP	-	expression tag	UNP O88738
B	-30	ASP	-	expression tag	UNP O88738
B	-29	ASP	-	expression tag	UNP O88738
B	-28	LYS	-	expression tag	UNP O88738
B	-27	ARG	-	expression tag	UNP O88738
B	-26	VAL	-	expression tag	UNP O88738
B	-25	VAL	-	expression tag	UNP O88738
B	-24	PRO	-	expression tag	UNP O88738
B	-23	LEU	-	expression tag	UNP O88738
B	-22	GLU	-	expression tag	UNP O88738
B	-21	SER	-	expression tag	UNP O88738
B	-20	THR	-	expression tag	UNP O88738
B	-19	GLY	-	expression tag	UNP O88738
B	-18	LEU	-	expression tag	UNP O88738
B	-17	GLN	-	expression tag	UNP O88738
B	-16	GLU	-	expression tag	UNP O88738
B	-15	LEU	-	expression tag	UNP O88738
B	-14	ALA	-	expression tag	UNP O88738
B	-13	THR	-	expression tag	UNP O88738
B	-12	MET	-	expression tag	UNP O88738
B	-11	GLU	-	expression tag	UNP O88738
B	-10	GLN	-	expression tag	UNP O88738
B	-9	LYS	-	expression tag	UNP O88738
B	-8	LEU	-	expression tag	UNP O88738
B	-7	ILE	-	expression tag	UNP O88738
B	-6	SER	-	expression tag	UNP O88738
B	-5	GLU	-	expression tag	UNP O88738
B	-4	GLU	-	expression tag	UNP O88738
B	-3	ASP	-	expression tag	UNP O88738
B	-2	LEU	-	expression tag	UNP O88738
B	-1	GLU	-	expression tag	UNP O88738

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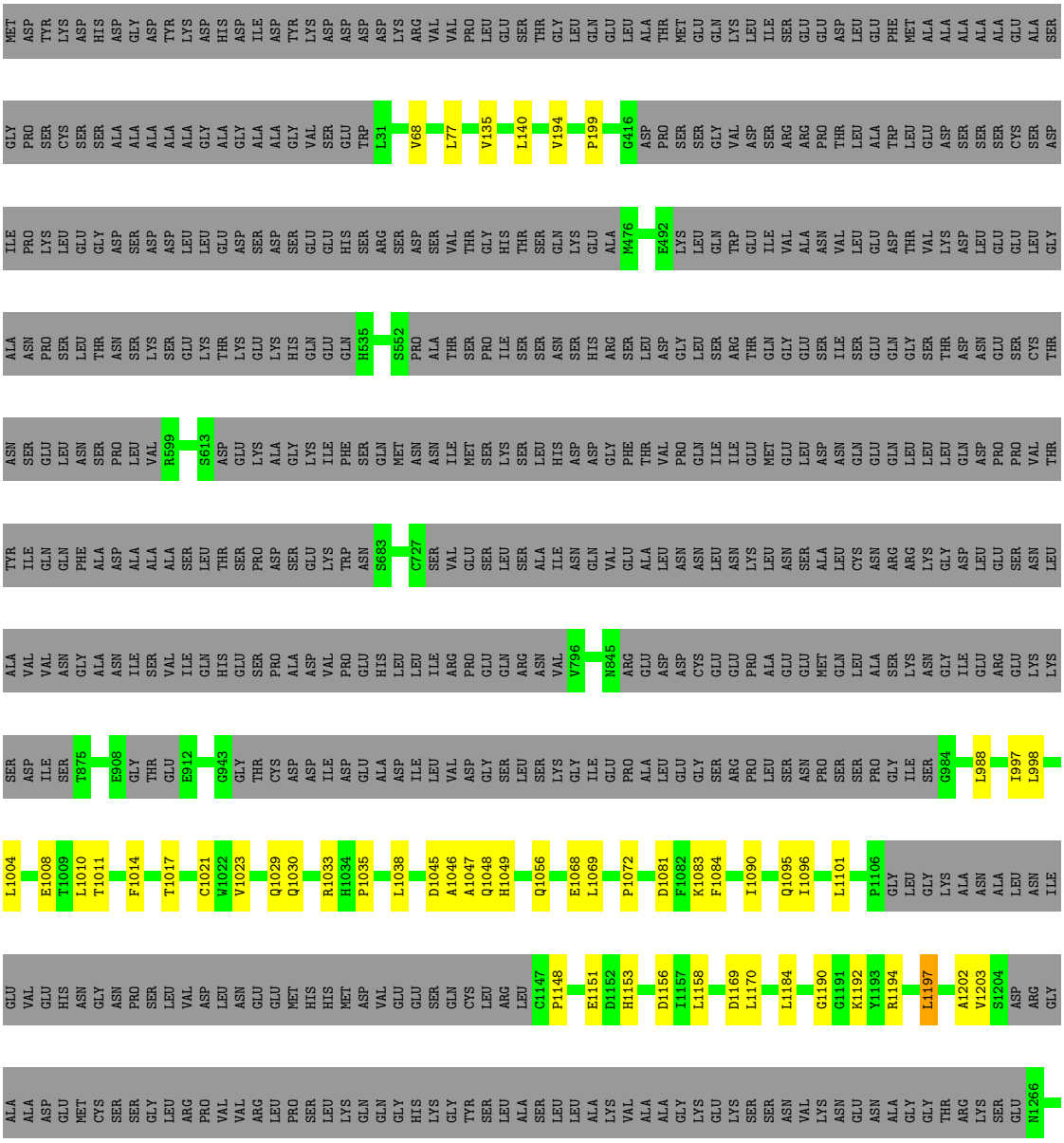
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP O88738
B	3226	THR	SER	conflict	UNP O88738
B	3914	VAL	MET	conflict	UNP O88738
B	3929	VAL	ILE	conflict	UNP O88738
B	4346	MET	VAL	conflict	UNP O88738

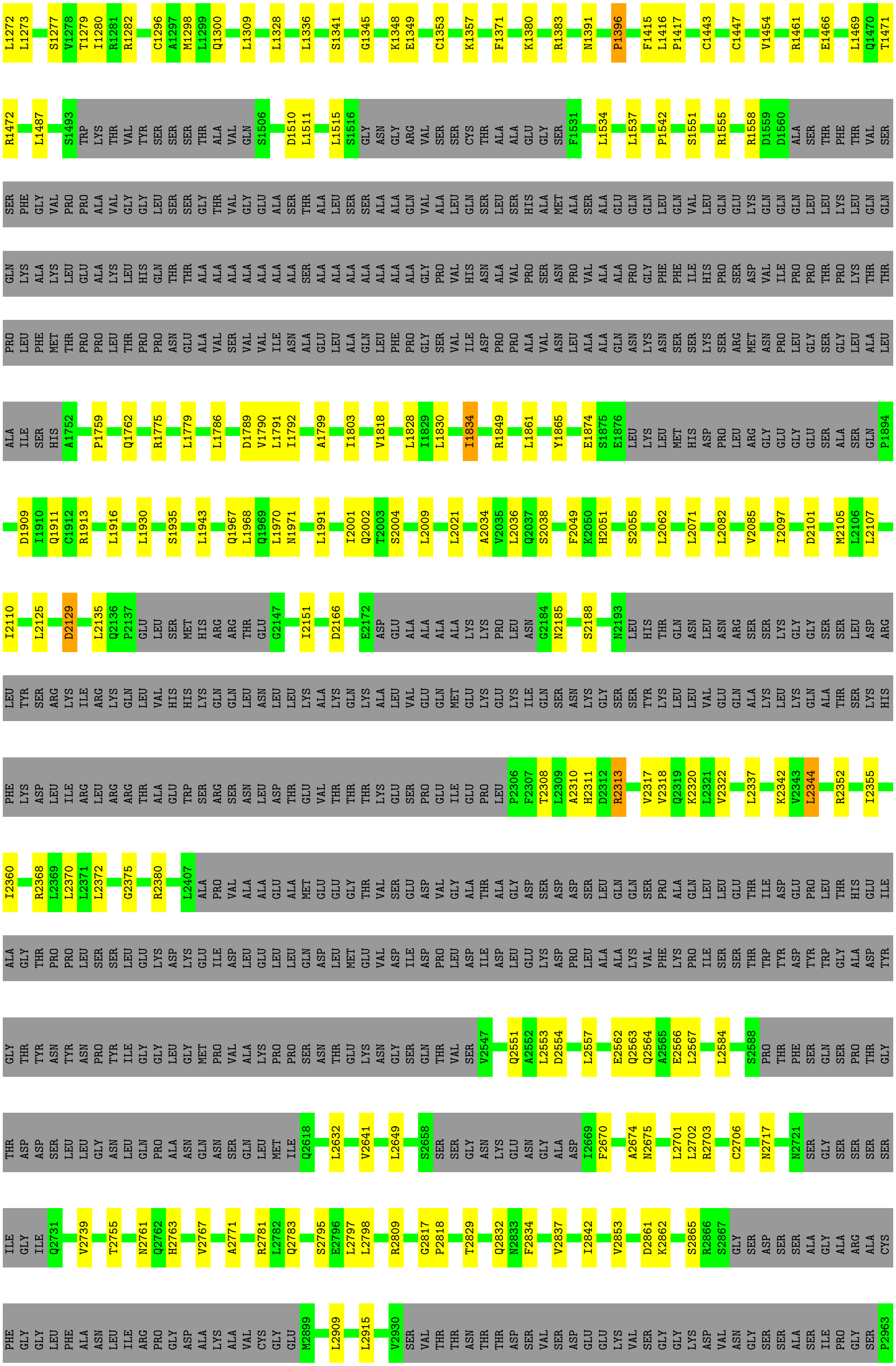
3 Residue-property plots (i)

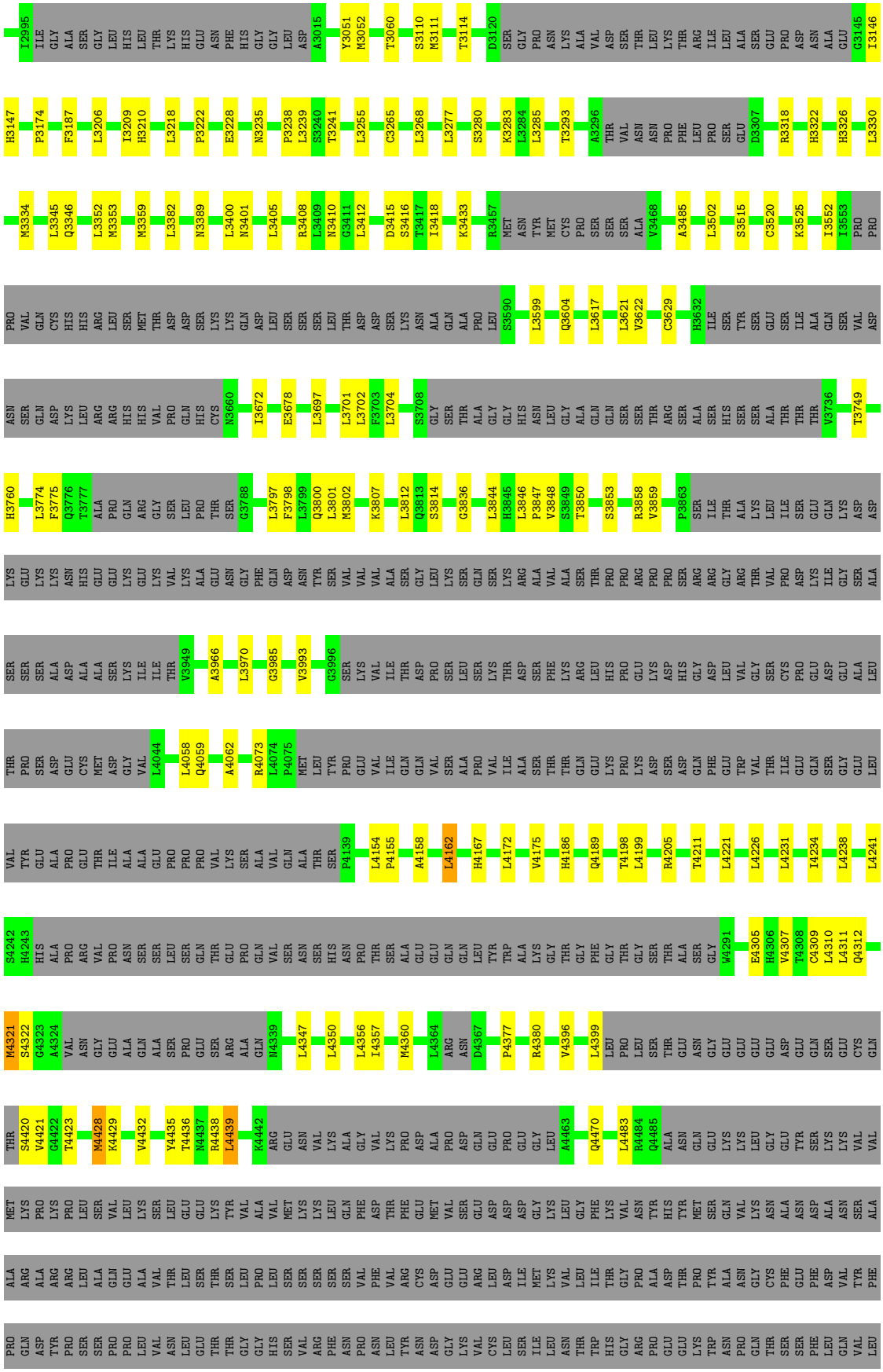
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

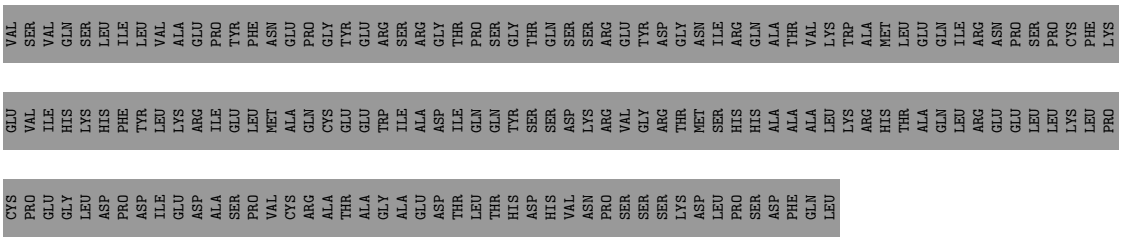
- Molecule 1: Isoform 2 of Baculoviral IAP repeat-containing protein 6

Chain A:



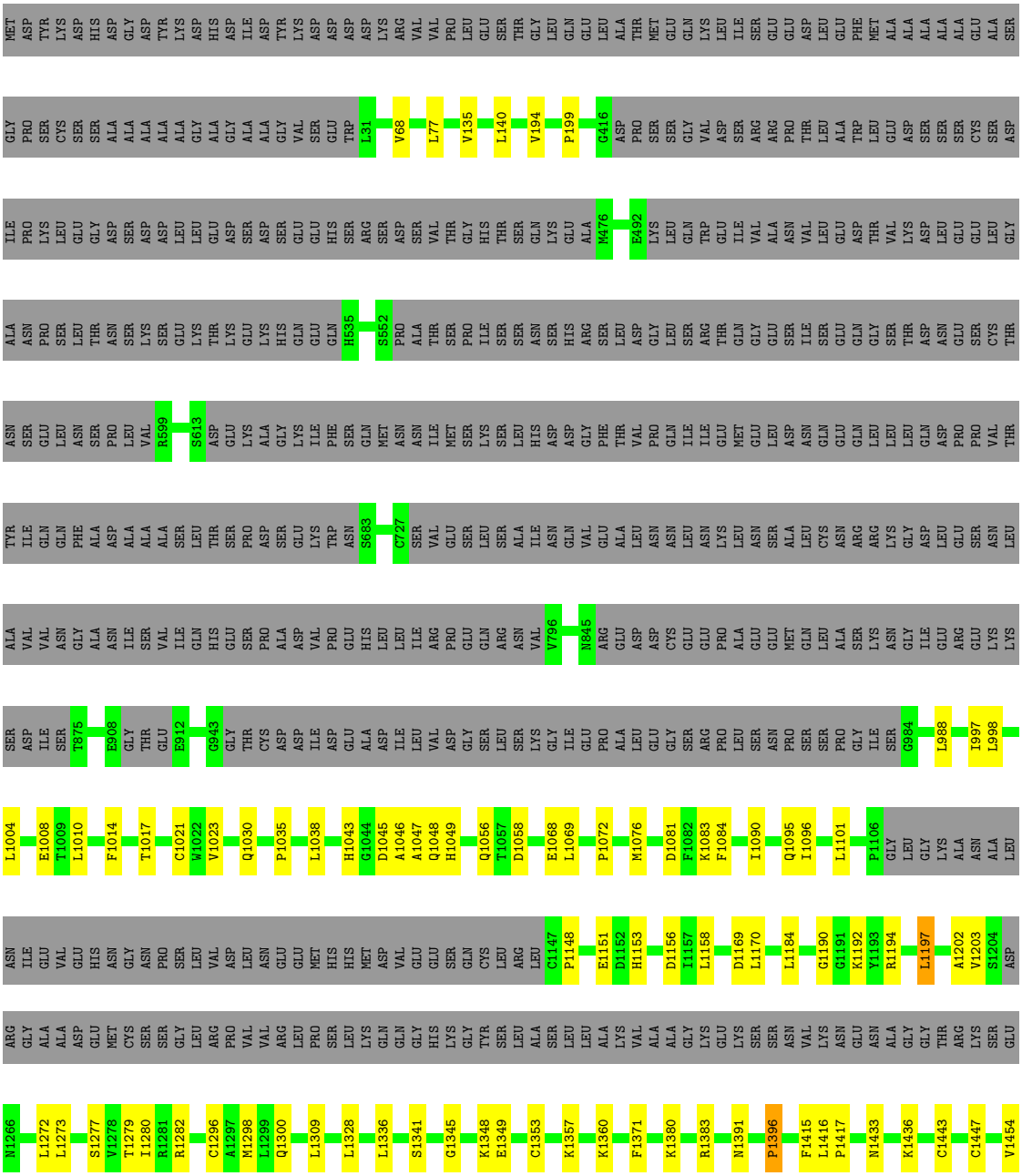

L1272 L1273 S1277 V1278 T1279 I1280 R1281 R1282 C1296 A1297 M1298 L1299 Q1300 L1309 L1328 L1336 S1341 G1345 K1348 E1349 C1353 K1357 F1371 K1380 R1383 N1391 P1396 F1415 L1416 P1417 C1443 C1447 V1454 R1461 E1466 L1469 Q1470 T1471
R1472 L1487 S1493 TRP LYS THR VAL TYR SER SER SER THR ALA VAL GLN S1506 D1510 L1511 L1515 S1516 GLY ASN GLY ARG VAL SER SER CYS THR ALA ALA GLU GLY SER F1531 L1534 L1537 P1542 S1551 R1555 R1558 D1559 D1560 ALA SER THR PHE THR VAL SER
SER PHE GLY VAL PRO PRO ALA VAL GLY GLY LEU SER SER GLY THR VAL GLY GLU ALA SER THR ALA LEU SER SER ALA ALA GLN VAL ALA LEU GLN SER LEU SER HIS ALA MET ALA SER ALA GLU GLN GLN LEU GLN VAL LEU GLN GLU LYS GLN GLN GLN LEU LEU LYS LEU GLN GLN
GLN LYS ALA LYS LEU GLU ALA LYS LEU HIS GLN THR THR ALA ALA ALA ALA ALA ALA ALA SER ALA ALA ALA ALA ALA ALA ALA GLY PRO VAL HIS ASN ALA VAL PRO SER ASN PRO VAL ALA ALA PRO GLY PHE PHE ILE HIS PRO SER ASP VAL ILE PRO PRO THR PRO LYS THR THR
PRO LEU PHE MET THR PRO PRO LEU THR PRO PRO ASN GLU ALA VAL SER VAL VAL ILE ASN ALA GLU LEU ALA GLN LEU PHE PRO GLY SER VAL ILE ASP PRO PRO ALA VAL ASN LEU ALA ALA GLN ASN LYS ASN SER SER LYS SER ARG MET ASN PRO LEU GLY SER GLY LEU ALA LEU
ALA ILE SER HIS A1752 P1759 Q1762 R1775 L1779 L1786 D1789 V1790 L1791 I1792 A1799 I1803 V1818 L1828 I1829 L1830 I1834 R1849 L1861 Y1865 E1874 S1875 E1876 LEU LYS LEU MET HIS ASP PRO LEU ARG GLY GLU GLY GLU SER ALA SER GLN P1894
D1909 I1910 Q1911 C1912 R1913 L1916 L1930 S1935 L1943 Q1967 L1968 Q1969 L1970 N1971 L1991 I2001 Q2002 T2003 S2004 L2009 L2021 A2034 V2035 L2036 Q2037 S2038 F2049 K2050 H2051 S2055 L2062 L2071 L2082 V2085 I2097 D2101 M2105 L2106 L2107
I2110 L2125 D2129 L2135 Q2136 P2137 GLU LEU SER MET HIS ARG ARG THR GLU G2147 I2151 D2166 E2172 ASP GLU ALA ALA ALA LYS PRO LEU ASN G2184 N2185 S2188 N2193 LEU HIS THR GLN ASN LEU ASN ARG SER SER LYS GLY GLY SER SER LEU ASP ARG
LEU TYR SER ARG LYS ILE ARG LYS GLN LEU VAL HIS HIS LYS GLN GLN LEU ASN LEU LEU LYS ALA LYS GLN LYS ALA LEU VAL GLU GLN MET GLU LYS GLU LYS ILE GLN SER ASN LYS GLY SER SER TYR LYS LEU LEU VAL GLU GLN ALA LYS SER LEU LYS GLN ALA THR SER LYS HIS
PHE LYS ASP LEU ILE ARG LEU ARG ARG THR ALA GLU TRP SER ARG SER ASN LEU ASP THR GLU VAL THR THR LYS GLU SER PRO GLU ILE GLU PRO LEU P2306 F2307 T2308 L2309 A2310 H2311 D2312 R2313 V2317 V2318 Q2319 K2320 L2321 V2322 L2337 K2342 V2343 L2344 R2352 I2355
I2360 R2368 L2369 L2370 L2371 L2372 G2375 R2380 L2407 ALA PRO VAL ALA ALA GLU ALA MET GLU GLU GLY THR VAL SER GLU ASP VAL GLY ALA THR ALA GLY ASP SER ASP ASP SER LEU GLN GLN SER PRO ALA GLN LEU LEU GLU THR ILE ASP GLU PRO LEU THR HIS GLU ILE
ALA GLY THR PRO PRO LEU SER SER LEU GLU LYS ASP LYS GLU ILE ASP LEU GLU LEU LEU GLN ASP LEU MET GLU VAL ASP ILE ASP PRO LEU ASP ILE ASP LEU GLU LYS ASP PRO LEU ALA ALA LYS VAL PHE LYS PRO ILE SER SER THR TRP TYR ASP TYR TRP GLY ALA ASP TYR
GLY THR TYR ASN TYR ASN PRO TYR ILE GLY GLY LEU GLY MET PRO VAL ALA LYS PRO PRO SER ASN THR GLU LYS ASN GLY SER GLN THR VAL SER V2547 Q2551 A2552 L2553 D2554 L2557 E2562 Q2563 Q2564 A2565 E2566 L2567 L2584 S2588 PRO THR PHE SER GLN SER PRO THR GLY
THR ASP ASP SER LEU LEU GLY ASN LEU GLN PRO ALA ASN GLN ASN SER GLN LEU MET ILE Q2618 L2632 V2641 L2649 S2658 SER SER GLY ASN LYS GLU ASN GLY ALA ASP I2669 F2670 A2674 N2675 L2701 L2702 R2703 C2706 N2717 N2721 SER GLY SER SER SER SER
ILE GLY ILE Q2731 V2739 T2755 N2761 Q2762 H2763 V2767 A2771 R2781 L2782 Q2783 S2795 E2796 L2797 L2798 R2809 G2817 P2818 T2829 Q2832 N2833 F2834 V2837 I2842 V2853 D2861 K2862 S2865 R2866 S2867 GLY SER ASP SER SER ALA GLY ALA ARG ALA CYS
PHE GLY GLY LEU PHE ALA ASN LEU ILE ARG PRO GLY ASP ALA LYS ALA VAL CYS GLY GLU M2899 L2909 L2915 V2930 SER VAL THR THR ASN THR THR ASP SER VAL SER ASP GLU GLU LYS VAL SER GLY GLY LYS ASP VAL ASN GLY SER SER ALA SER ILE PRO GLY SER P2963

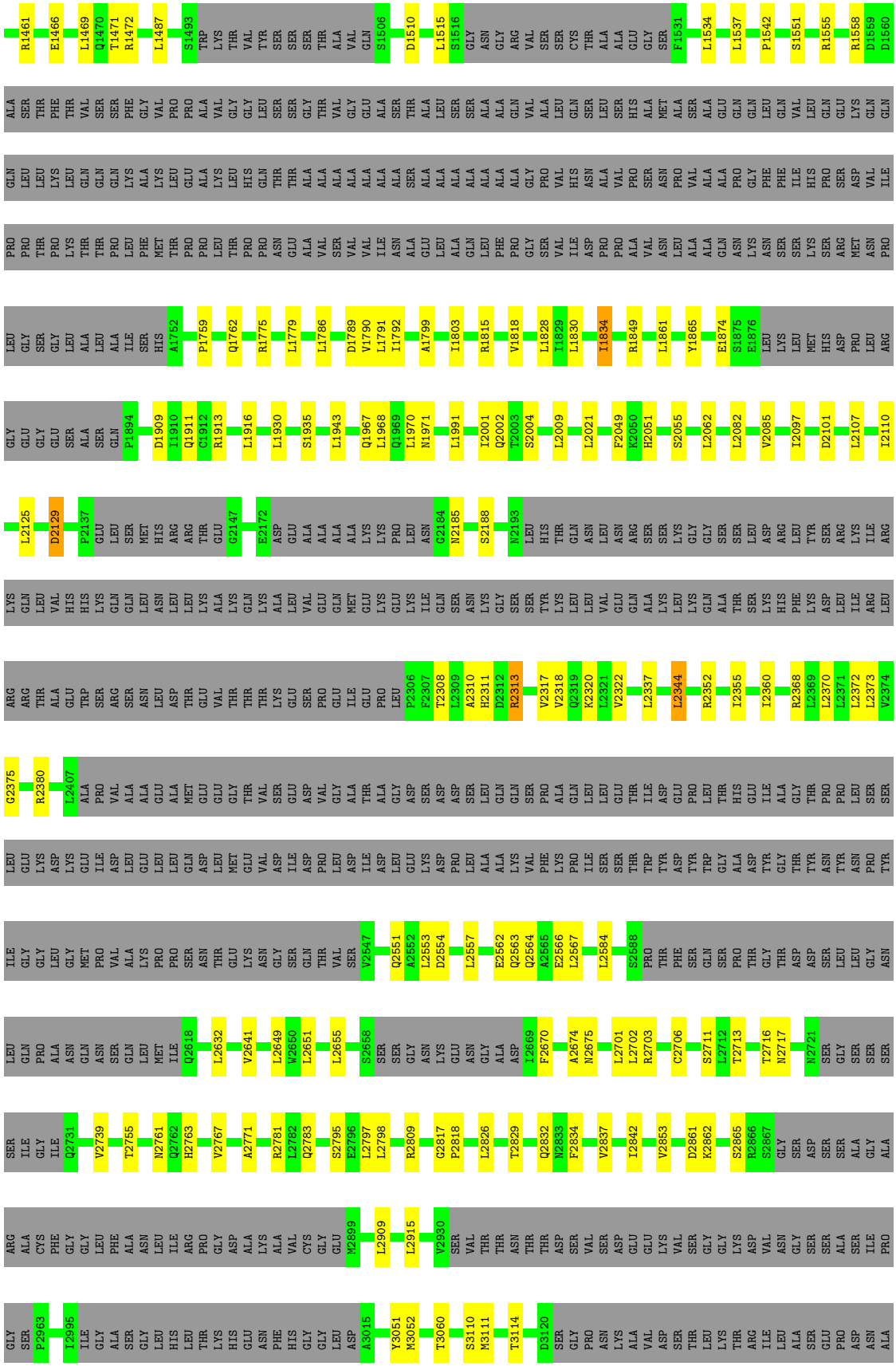


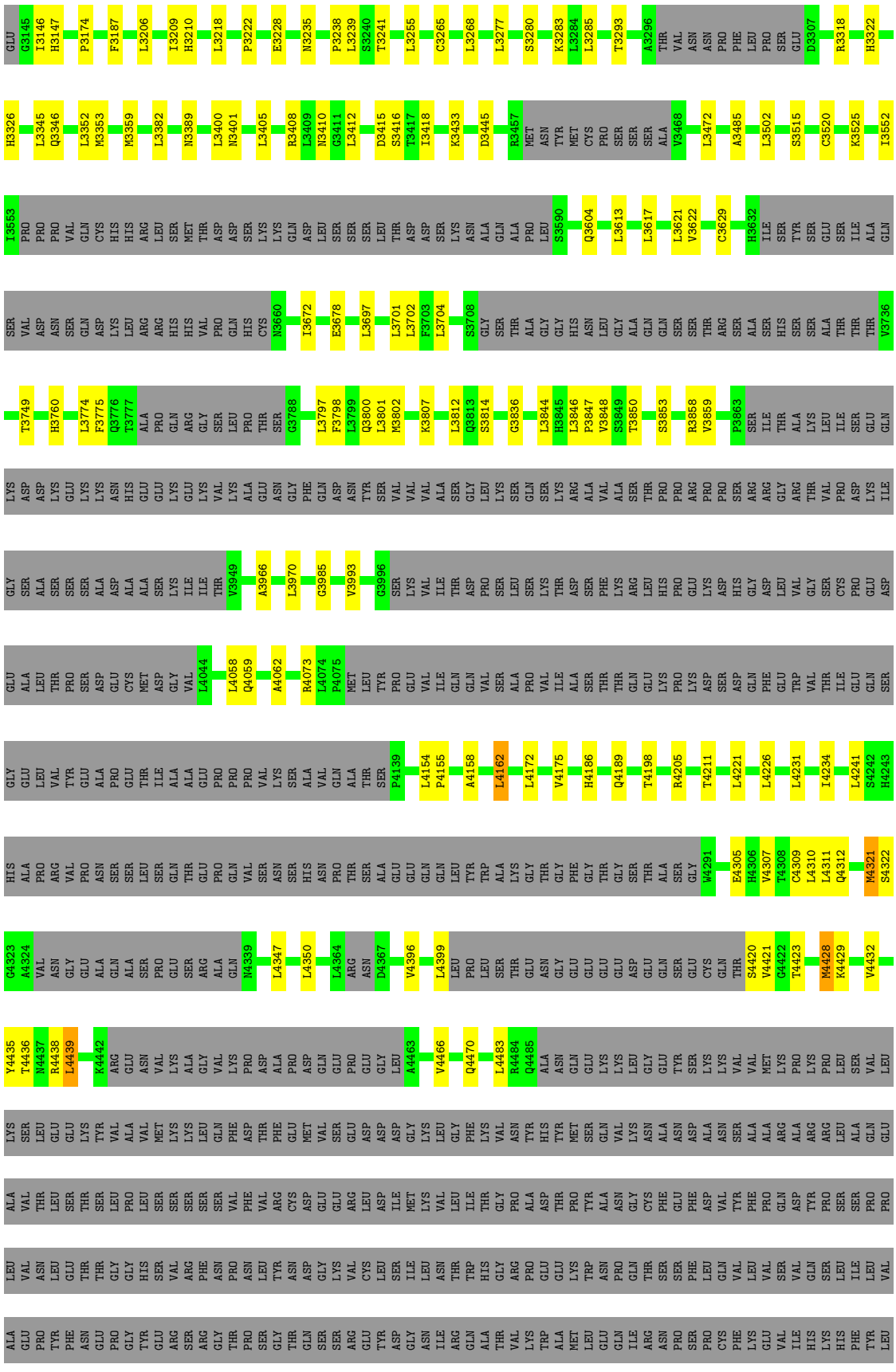


• Molecule 1: Isoform 2 of Baculoviral IAP repeat-containing protein 6

Chain B:








LYS ARG ILE GLU LEU MET ALA GLN CYS GLU GLU TRP ILE ALA ASP ILE GLN GLN TYR SER SER ASP LYS ARG VAL GLY ARG THR MET SER HIS HIS ALA ALA ALA LEU LYS ARG HIS THR ALA GLN LEU ARG GLU GLU LEU LEU LYS LEU PRO CYS PRO GLU GLY LEU ASP PRO ASP ILE


GLU ASP ALA SER PRO VAL CYS ARG ALA THR ALA GLY ALA GLU ASP THR LEU THR HIS ASP HIS VAL ASN PRO SER SER SER LYS ASP LEU PRO SER ASP PHE GLN LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	68.4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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	0.29	0/21276	0.60	14/28980 (0.0%)
1	B	0.29	0/21276	0.60	14/28980 (0.0%)
All	All	0.29	0/42552	0.60	28/57960 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4162	LEU	CB-CG-CD2	-9.11	95.51	111.00
1	B	4162	LEU	CB-CG-CD2	-9.10	95.53	111.00
1	A	2337	LEU	CA-CB-CG	7.63	132.86	115.30
1	B	2337	LEU	CA-CB-CG	7.62	132.83	115.30
1	B	2129	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	2129	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	4241	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	4241	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	4321	MET	CA-CB-CG	6.76	124.79	113.30
1	B	4321	MET	CA-CB-CG	6.73	124.75	113.30
1	A	1004	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	1004	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	1396	PRO	CA-N-CD	-5.59	103.67	111.50
1	A	1396	PRO	CA-N-CD	-5.57	103.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4439	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	4439	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	1004	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	1004	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	1197	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	1197	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	2372	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	2372	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	4305	GLU	CA-CB-CG	5.08	124.57	113.40
1	B	4428	MET	CG-SD-CE	-5.07	92.08	100.20
1	A	4428	MET	CG-SD-CE	-5.07	92.09	100.20
1	B	4305	GLU	CA-CB-CG	5.06	124.54	113.40
1	B	2344	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	2344	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396	PRO	Peptide
1	A	1834	ILE	Peptide
1	B	1396	PRO	Peptide
1	B	1834	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20950	0	19684	210	0
1	B	20950	0	19684	211	0
All	All	41900	0	39368	396	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 5.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3798:PHE:O	1:B:3802:MET:HB3	1.81	0.81
1:A:3798:PHE:O	1:A:3802:MET:HB3	1.81	0.80
1:B:1383:ARG:HH21	1:B:2562:GLU:HB2	1.52	0.74
1:A:1383:ARG:HH21	1:A:2562:GLU:HB2	1.52	0.73
1:A:2375:GLY:HA2	1:A:2641:VAL:HA	1.76	0.68
1:A:1349:GLU:O	1:A:1353:CYS:HB2	1.94	0.67
1:B:2375:GLY:HA2	1:B:2641:VAL:HA	1.76	0.67
1:B:1349:GLU:O	1:B:1353:CYS:HB2	1.94	0.66
1:A:1417:PRO:HG2	1:A:2001:ILE:HG12	1.78	0.65
1:B:1417:PRO:HG2	1:B:2001:ILE:HG12	1.78	0.65
1:A:2703:ARG:NH1	1:A:2706:CYS:SG	2.71	0.64
1:B:1298:MET:HG2	1:B:1336:LEU:HD21	1.80	0.64
1:B:2703:ARG:NH1	1:B:2706:CYS:SG	2.71	0.63
1:B:3353:MET:SD	1:B:3408:ARG:NH2	2.72	0.63
1:A:3353:MET:SD	1:A:3408:ARG:NH2	2.72	0.63
1:A:1298:MET:HG2	1:A:1336:LEU:HD21	1.80	0.62
1:B:1169:ASP:HA	1:B:2567:LEU:HD21	1.83	0.61
1:B:1789:ASP:HB2	1:B:1865:TYR:HB2	1.82	0.60
1:A:1169:ASP:HA	1:A:2567:LEU:HD21	1.83	0.60
1:B:3807:LYS:HE2	1:B:3847:PRO:HG3	1.83	0.60
1:A:4432:VAL:HG11	1:A:4470:GLN:HB2	1.84	0.60
1:A:3702:LEU:HD13	1:A:3774:LEU:HD22	1.83	0.60
1:A:3807:LYS:HE2	1:A:3847:PRO:HG3	1.83	0.60
1:A:4420:SER:N	1:A:4423:THR:HG1	2.00	0.60
1:A:1789:ASP:HB2	1:A:1865:TYR:HB2	1.82	0.60
1:A:1792:ILE:HB	1:A:1828:LEU:HB3	1.84	0.60
1:A:4198:THR:OG1	1:A:4309:CYS:SG	2.60	0.60
1:A:1443:CYS:O	1:A:1447:CYS:HB2	2.02	0.59
1:B:1341:SER:HB2	1:B:1391:ASN:HD22	1.67	0.59
1:B:4432:VAL:HG11	1:B:4470:GLN:HB2	1.84	0.59
1:B:3228:GLU:HB2	1:B:3265:CYS:HB3	1.84	0.59
1:B:4420:SER:N	1:B:4423:THR:HG1	2.00	0.59
1:B:2310:ALA:HB3	1:B:2313:ARG:HE	1.68	0.59
1:B:4198:THR:OG1	1:B:4309:CYS:SG	2.60	0.59
1:B:3702:LEU:HD13	1:B:3774:LEU:HD22	1.83	0.59
1:B:3206:LEU:HD21	1:B:3209:ILE:HD11	1.85	0.59
1:A:3228:GLU:HB2	1:A:3265:CYS:HB3	1.84	0.59
1:A:1341:SER:HB2	1:A:1391:ASN:HD22	1.67	0.58
1:A:2310:ALA:HB3	1:A:2313:ARG:HE	1.68	0.58
1:A:4234:ILE:HG23	1:A:4310:LEU:HD23	1.86	0.58
1:A:3206:LEU:HD21	1:A:3209:ILE:HD11	1.85	0.58
1:B:1443:CYS:O	1:B:1447:CYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4234:ILE:HG23	1:B:4310:LEU:HD23	1.86	0.58
1:B:4307:VAL:O	1:B:4311:LEU:HB3	2.04	0.58
1:B:1170:LEU:HD11	1:B:2551:GLN:HG2	1.86	0.58
1:B:1967:GLN:O	1:B:1971:ASN:ND2	2.37	0.58
1:A:1035:PRO:HD2	1:A:1038:LEU:HD12	1.86	0.58
1:A:1170:LEU:HD11	1:A:2551:GLN:HG2	1.86	0.58
1:B:1792:ILE:HB	1:B:1828:LEU:HB3	1.84	0.58
1:A:1967:GLN:O	1:A:1971:ASN:ND2	2.37	0.58
1:A:2308:THR:HG21	1:A:2352:ARG:HH21	1.69	0.57
1:B:4396:VAL:HG13	1:B:4483:LEU:HD13	1.87	0.57
1:A:2703:ARG:HE	1:B:3238:PRO:HB2	1.70	0.56
1:B:1035:PRO:HD2	1:B:1038:LEU:HD12	1.86	0.56
1:A:1534:LEU:HB3	1:A:1537:LEU:HD21	1.87	0.56
1:A:4307:VAL:O	1:A:4311:LEU:HB3	2.04	0.56
1:B:1345:GLY:H	1:B:1348:LYS:HD3	1.70	0.56
1:A:1017:THR:OG1	1:A:1068:GLU:OE2	2.23	0.56
1:A:1014:PHE:HA	1:A:1072:PRO:HD3	1.88	0.56
1:A:1190:GLY:HA3	1:A:1192:LYS:HE3	1.88	0.56
1:A:2809:ARG:O	1:B:2809:ARG:NH2	2.39	0.56
1:B:2370:LEU:HD22	1:B:2649:LEU:HD21	1.87	0.56
1:A:2809:ARG:NH2	1:B:2809:ARG:O	2.39	0.56
1:A:4396:VAL:HG13	1:A:4483:LEU:HD13	1.87	0.56
1:B:1014:PHE:HA	1:B:1072:PRO:HD3	1.88	0.56
1:B:1190:GLY:HA3	1:B:1192:LYS:HE3	1.88	0.55
1:A:2370:LEU:HD22	1:A:2649:LEU:HD21	1.87	0.55
1:B:2308:THR:HG21	1:B:2352:ARG:HH21	1.70	0.55
1:A:2185:ASN:HB2	1:A:2188:SER:HB3	1.88	0.55
1:A:4321:MET:SD	1:A:4322:SER:N	2.76	0.55
1:B:1017:THR:OG1	1:B:1068:GLU:OE2	2.23	0.55
1:B:3239:LEU:HD13	1:B:3255:LEU:HD21	1.89	0.55
1:B:4321:MET:SD	1:B:4322:SER:N	2.76	0.55
1:A:1008:GLU:OE2	1:A:1282:ARG:NH1	2.40	0.55
1:A:2101:ASP:OD1	1:A:2101:ASP:N	2.37	0.55
1:A:3238:PRO:HB2	1:B:2703:ARG:HE	1.70	0.55
1:A:1345:GLY:H	1:A:1348:LYS:HD3	1.70	0.55
1:B:1021:CYS:O	1:B:1056:GLN:NE2	2.40	0.55
1:B:1534:LEU:HB3	1:B:1537:LEU:HD21	1.87	0.55
1:B:2675:ASN:OD1	1:B:2781:ARG:NH1	2.40	0.55
1:B:1558:ARG:HA	1:B:1762:GLN:HA	1.89	0.55
1:A:1461:ARG:NH2	1:A:2002:GLN:O	2.39	0.55
1:A:2675:ASN:OD1	1:A:2781:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:GLU:OE2	1:B:1282:ARG:NH1	2.40	0.55
1:B:1461:ARG:NH2	1:B:2002:GLN:O	2.39	0.55
1:A:1461:ARG:NH2	1:A:2004:SER:O	2.40	0.54
1:A:1558:ARG:HA	1:A:1762:GLN:HA	1.89	0.54
1:A:1021:CYS:O	1:A:1056:GLN:NE2	2.40	0.54
1:A:2761:ASN:ND2	1:B:2865:SER:O	2.41	0.54
1:A:3239:LEU:HD13	1:A:3255:LEU:HD21	1.89	0.54
1:A:3412:LEU:HD21	1:B:1935:SER:HB2	1.90	0.54
1:A:4154:LEU:HD12	1:A:4155:PRO:HD2	1.90	0.54
1:B:1461:ARG:NH2	1:B:2004:SER:O	2.40	0.54
1:B:1084:PHE:HB2	1:B:1273:LEU:HD22	1.90	0.54
1:B:2185:ASN:HB2	1:B:2188:SER:HB3	1.88	0.54
1:B:3853:SER:HB2	1:B:3966:ALA:HB1	1.90	0.54
1:A:2755:THR:HB	1:A:2817:GLY:H	1.73	0.53
1:B:3345:LEU:HD12	1:B:3382:LEU:HD13	1.91	0.53
1:A:3621:LEU:HD23	1:A:3672:ILE:HG23	1.91	0.53
1:A:1935:SER:HB2	1:B:3412:LEU:HD21	1.91	0.53
1:A:1799:ALA:HB2	1:A:1849:ARG:HA	1.91	0.53
1:A:2865:SER:O	1:B:2761:ASN:ND2	2.41	0.53
1:A:3345:LEU:HD12	1:A:3382:LEU:HD13	1.91	0.53
1:A:4186:HIS:HB2	1:A:4189:GLN:HG2	1.90	0.53
1:B:1799:ALA:HB2	1:B:1849:ARG:HA	1.91	0.53
1:B:3621:LEU:HD23	1:B:3672:ILE:HG23	1.91	0.53
1:B:4186:HIS:HB2	1:B:4189:GLN:HG2	1.90	0.53
1:A:3797:LEU:O	1:A:3801:LEU:HB3	2.09	0.52
1:B:4154:LEU:HD12	1:B:4155:PRO:HD2	1.90	0.52
1:B:2755:THR:HB	1:B:2817:GLY:H	1.73	0.52
1:B:3797:LEU:O	1:B:3801:LEU:HB3	2.09	0.52
1:A:1084:PHE:HB2	1:A:1273:LEU:HD22	1.90	0.52
1:A:3400:LEU:HD13	1:B:2368:ARG:HG2	1.92	0.52
1:A:4435:TYR:HA	1:A:4438:ARG:HD2	1.92	0.52
1:A:2368:ARG:HG2	1:B:3400:LEU:HD13	1.92	0.52
1:A:3241:THR:OG1	1:B:2763:HIS:ND1	2.43	0.52
1:A:3853:SER:HB2	1:A:3966:ALA:HB1	1.90	0.52
1:B:3433:LYS:HG3	1:B:3502:LEU:HD21	1.92	0.52
1:A:2763:HIS:ND1	1:B:3241:THR:OG1	2.43	0.52
1:B:4435:TYR:HA	1:B:4438:ARG:HD2	1.92	0.52
1:A:3235:ASN:ND2	1:B:2670:PHE:O	2.39	0.52
1:B:3798:PHE:O	1:B:3802:MET:CB	2.57	0.52
1:A:2767:VAL:HG13	1:A:2818:PRO:HB3	1.92	0.51
1:B:1510:ASP:OD1	1:B:1510:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3622:VAL:HG23	1:B:3697:LEU:HD22	1.92	0.51
1:A:1030:GLN:HE22	1:A:1047:ALA:HB3	1.76	0.51
1:B:2703:ARG:HH12	1:B:2771:ALA:HB2	1.75	0.51
1:A:1510:ASP:N	1:A:1510:ASP:OD1	2.43	0.51
1:B:3322:HIS:O	1:B:3326:HIS:HB2	2.11	0.51
1:B:2767:VAL:HG13	1:B:2818:PRO:HB3	1.92	0.51
1:A:2049:PHE:HE1	1:A:2085:VAL:HG11	1.76	0.51
1:A:2674:ALA:O	1:A:2717:ASN:ND2	2.41	0.51
1:A:2703:ARG:HH12	1:A:2771:ALA:HB2	1.75	0.51
1:A:3622:VAL:HG23	1:A:3697:LEU:HD22	1.92	0.51
1:A:3415:ASP:HA	1:A:3418:ILE:HD12	1.93	0.51
1:A:3433:LYS:HG3	1:A:3502:LEU:HD21	1.92	0.51
1:B:1030:GLN:HE22	1:B:1047:ALA:HB3	1.75	0.51
1:A:3322:HIS:O	1:A:3326:HIS:HB2	2.11	0.50
1:B:3415:ASP:HA	1:B:3418:ILE:HD12	1.93	0.50
1:A:3401:ASN:OD1	1:B:2368:ARG:NH2	2.45	0.50
1:B:2101:ASP:OD1	1:B:2101:ASP:N	2.37	0.50
1:A:1309:LEU:HD21	1:A:1357:LYS:HB3	1.94	0.50
1:B:2125:LEU:HB3	1:B:2317:VAL:HG21	1.93	0.50
1:B:3389:ASN:HA	1:B:3410:ASN:HD21	1.76	0.50
1:A:1454:VAL:HG13	1:A:2009:LEU:HD22	1.94	0.50
1:B:4062:ALA:HB1	1:B:4158:ALA:HB1	1.94	0.50
1:A:3604:GLN:NE2	1:A:3678:GLU:O	2.45	0.50
1:A:4226:LEU:HD11	1:A:4347:LEU:HD23	1.94	0.50
1:B:1296:CYS:O	1:B:1300:GLN:HB2	2.12	0.50
1:A:3389:ASN:HA	1:A:3410:ASN:HD21	1.76	0.50
1:B:2049:PHE:HE1	1:B:2085:VAL:HG11	1.76	0.50
1:B:1790:VAL:HB	1:B:1830:LEU:HB2	1.93	0.49
1:A:1296:CYS:O	1:A:1300:GLN:HB2	2.12	0.49
1:B:4226:LEU:HD11	1:B:4347:LEU:HD23	1.94	0.49
1:A:2701:LEU:HD12	1:B:2862:LYS:HE2	1.95	0.49
1:A:4231:LEU:HA	1:A:4234:ILE:HD12	1.95	0.49
1:A:1010:LEU:HD13	1:A:1280:ILE:HG22	1.94	0.49
1:B:3210:HIS:HB2	1:B:3283:LYS:HB2	1.95	0.49
1:A:2125:LEU:HB3	1:A:2317:VAL:HG21	1.93	0.49
1:A:2368:ARG:NH2	1:B:3401:ASN:OD1	2.45	0.49
1:A:2861:ASP:OD1	1:A:2861:ASP:N	2.45	0.49
1:B:1309:LEU:HD21	1:B:1357:LYS:HB3	1.94	0.49
1:B:1466:GLU:HA	1:B:1469:LEU:HD12	1.94	0.49
1:B:2051:HIS:O	1:B:2055:SER:OG	2.31	0.49
1:B:2107:LEU:HA	1:B:2110:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3210:HIS:HB2	1:A:3283:LYS:HB2	1.95	0.49
1:B:1010:LEU:HD13	1:B:1280:ILE:HG22	1.94	0.49
1:A:2862:LYS:HE2	1:B:2701:LEU:HD12	1.95	0.49
1:A:3848:VAL:HA	1:A:3970:LEU:HB2	1.95	0.49
1:A:2563:GLN:OE1	1:A:2564:GLN:NE2	2.46	0.49
1:A:4062:ALA:HB1	1:A:4158:ALA:HB1	1.94	0.49
1:A:2739:VAL:HG13	1:A:2797:LEU:HD22	1.94	0.49
1:B:2861:ASP:OD1	1:B:2861:ASP:N	2.45	0.49
1:B:4231:LEU:HA	1:B:4234:ILE:HD12	1.94	0.49
1:A:3346:GLN:HB3	1:A:3405:LEU:HG	1.95	0.48
1:B:2129:ASP:O	1:B:2320:LYS:NZ	2.42	0.48
1:B:3515:SER:O	1:B:3525:LYS:NZ	2.44	0.48
1:A:1790:VAL:HB	1:A:1830:LEU:HB2	1.93	0.48
1:B:4347:LEU:HA	1:B:4350:LEU:HG	1.96	0.48
1:A:1466:GLU:HA	1:A:1469:LEU:HD12	1.94	0.48
1:A:1471:THR:HG21	1:A:2097:ILE:HG22	1.95	0.48
1:A:2051:HIS:O	1:A:2055:SER:OG	2.31	0.48
1:B:2563:GLN:OE1	1:B:2564:GLN:NE2	2.46	0.48
1:A:1909:ASP:OD2	1:A:1913:ARG:NH1	2.47	0.48
1:B:1454:VAL:HG13	1:B:2009:LEU:HD22	1.94	0.48
1:B:1471:THR:HG21	1:B:2097:ILE:HG22	1.95	0.48
1:B:1909:ASP:OD2	1:B:1913:ARG:NH1	2.47	0.48
1:B:2739:VAL:HG13	1:B:2797:LEU:HD22	1.94	0.48
1:B:3814:SER:HB2	1:B:3993:VAL:HB	1.95	0.48
1:A:3798:PHE:O	1:A:3802:MET:CB	2.57	0.48
1:A:1383:ARG:NH1	1:A:2566:GLU:OE1	2.47	0.48
1:A:3060:THR:O	1:B:2380:ARG:NH1	2.46	0.48
1:B:1383:ARG:NH1	1:B:2566:GLU:OE1	2.47	0.47
1:B:3346:GLN:HB3	1:B:3405:LEU:HG	1.95	0.47
1:B:1551:SER:O	1:B:1555:ARG:NH1	2.48	0.47
1:B:3604:GLN:NE2	1:B:3678:GLU:O	2.45	0.47
1:A:2380:ARG:NH1	1:B:3060:THR:O	2.47	0.47
1:B:2129:ASP:HB3	1:B:2317:VAL:HG22	1.97	0.47
1:A:3174:PRO:HG2	1:A:3280:SER:HB3	1.95	0.47
1:B:1786:LEU:HD21	1:B:1874:GLU:HB3	1.97	0.47
1:A:3218:LEU:HB2	1:B:3218:LEU:HB2	1.95	0.47
1:B:1058:ASP:OD2	1:B:1058:ASP:N	2.48	0.47
1:A:1551:SER:O	1:A:1555:ARG:NH1	2.47	0.47
1:A:1786:LEU:HD21	1:A:1874:GLU:HB3	1.97	0.47
1:A:2107:LEU:HA	1:A:2110:ILE:HG22	1.94	0.47
1:B:3812:LEU:HD22	1:B:3859:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3812:LEU:HD22	1:A:3859:VAL:HG11	1.96	0.47
1:A:4347:LEU:HA	1:A:4350:LEU:HG	1.96	0.47
1:B:3110:SER:OG	1:B:3111:MET:N	2.46	0.47
1:B:3848:VAL:HA	1:B:3970:LEU:HB2	1.95	0.47
1:A:3760:HIS:HD2	1:A:3985:GLY:HA3	1.79	0.47
1:B:3174:PRO:HG2	1:B:3280:SER:HB3	1.95	0.47
1:A:2670:PHE:O	1:B:3235:ASN:ND2	2.39	0.47
1:A:3520:CYS:HA	1:A:3525:LYS:HD3	1.96	0.47
1:B:3520:CYS:HA	1:B:3525:LYS:HD3	1.96	0.47
1:B:3775:PHE:O	1:B:4073:ARG:NH1	2.47	0.47
1:A:2842:ILE:HG23	1:A:2915:LEU:HD13	1.97	0.46
1:A:3775:PHE:O	1:A:4073:ARG:NH1	2.47	0.46
1:A:3814:SER:HB2	1:A:3993:VAL:HB	1.96	0.46
1:A:1911:GLN:HG3	1:A:1970:LEU:HD11	1.98	0.46
1:B:1096:ILE:HA	1:B:1202:ALA:HA	1.98	0.46
1:B:3760:HIS:HD2	1:B:3985:GLY:HA3	1.79	0.46
1:A:2129:ASP:HB3	1:A:2317:VAL:HG22	1.97	0.46
1:A:2553:LEU:HD23	1:A:2567:LEU:HD13	1.97	0.46
1:B:3629:CYS:HA	1:B:3704:LEU:HD13	1.98	0.46
1:B:2837:VAL:HG13	1:B:2842:ILE:HD11	1.97	0.46
1:B:1081:ASP:HB2	1:B:1279:THR:HB	1.98	0.46
1:A:2837:VAL:HG13	1:A:2842:ILE:HD11	1.97	0.46
1:B:1911:GLN:HG3	1:B:1970:LEU:HD11	1.98	0.46
1:B:2842:ILE:HG23	1:B:2915:LEU:HD13	1.97	0.46
1:B:4172:LEU:HA	1:B:4175:VAL:HG12	1.98	0.46
1:B:1045:ASP:HA	1:B:1048:GLN:HG3	1.98	0.46
1:A:1045:ASP:HA	1:A:1048:GLN:HG3	1.98	0.45
1:A:1046:ALA:HA	1:A:1049:HIS:CD2	2.51	0.45
1:A:4172:LEU:HA	1:A:4175:VAL:HG12	1.98	0.45
1:B:1076:MET:SD	1:B:1076:MET:N	2.87	0.45
1:A:2129:ASP:O	1:A:2320:LYS:NZ	2.42	0.45
1:A:3802:MET:HG3	1:A:4058:LEU:HD13	1.98	0.45
1:A:1096:ILE:HA	1:A:1202:ALA:HA	1.98	0.45
1:B:1153:HIS:HB3	1:B:1156:ASP:HB2	1.98	0.45
1:B:4428:MET:HB2	1:B:4428:MET:HE2	1.83	0.45
1:A:1081:ASP:HB2	1:A:1279:THR:HB	1.98	0.45
1:A:1014:PHE:HE1	1:A:1069:LEU:HD22	1.81	0.45
1:B:1046:ALA:HA	1:B:1049:HIS:CD2	2.51	0.45
1:A:3110:SER:OG	1:A:3111:MET:N	2.46	0.45
1:A:3222:PRO:HG3	1:A:3268:LEU:HD23	1.99	0.45
1:B:1534:LEU:HD23	1:B:1791:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3515:SER:O	1:A:3525:LYS:NZ	2.44	0.45
1:B:68:VAL:O	1:B:77:LEU:N	2.45	0.45
1:B:1095:GLN:O	1:B:1203:VAL:N	2.50	0.45
1:A:1153:HIS:HB3	1:A:1156:ASP:HB2	1.98	0.45
1:A:1534:LEU:HD23	1:A:1791:LEU:HD13	1.98	0.45
1:B:2553:LEU:HD23	1:B:2567:LEU:HD13	1.97	0.45
1:A:1095:GLN:O	1:A:1203:VAL:N	2.49	0.45
1:A:3629:CYS:HA	1:A:3704:LEU:HD13	1.98	0.45
1:B:2674:ALA:O	1:B:2717:ASN:ND2	2.41	0.45
1:B:3802:MET:HG3	1:B:4058:LEU:HD13	1.98	0.45
1:A:3187:PHE:HE2	1:A:3277:LEU:HB2	1.83	0.44
1:A:3485:ALA:HB1	1:A:3836:GLY:HA2	2.00	0.44
1:B:2557:LEU:HD21	1:B:2566:GLU:HB3	1.99	0.44
1:B:4307:VAL:O	1:B:4311:LEU:CB	2.65	0.44
1:B:4399:LEU:HB2	1:B:4421:VAL:HB	1.99	0.44
1:A:1779:LEU:HD21	1:A:1861:LEU:HD11	2.00	0.44
1:A:4307:VAL:O	1:A:4311:LEU:CB	2.65	0.44
1:B:3485:ALA:HB1	1:B:3836:GLY:HA2	1.99	0.44
1:B:3844:LEU:HD13	1:B:3858:ARG:HD2	2.00	0.44
1:A:2322:VAL:HG21	1:A:2360:ILE:HG12	2.00	0.44
1:B:3222:PRO:HG3	1:B:3268:LEU:HD23	1.99	0.44
1:A:1023:VAL:HG13	1:A:1056:GLN:HE22	1.82	0.44
1:A:3844:LEU:HD13	1:A:3858:ARG:HD2	1.99	0.44
1:B:1014:PHE:HE1	1:B:1069:LEU:HD22	1.81	0.44
1:B:1101:LEU:HB2	1:B:1197:LEU:HB2	1.99	0.44
1:A:3147:HIS:HE1	1:A:3293:THR:O	2.01	0.44
1:B:1779:LEU:HD21	1:B:1861:LEU:HD11	2.00	0.44
1:B:4059:GLN:HA	1:B:4162:LEU:HD21	1.99	0.44
1:A:4059:GLN:HA	1:A:4162:LEU:HD21	1.99	0.44
1:A:4399:LEU:HB2	1:A:4421:VAL:HB	1.99	0.44
1:B:1023:VAL:HG13	1:B:1056:GLN:HE22	1.82	0.44
1:B:3187:PHE:HE2	1:B:3277:LEU:HB2	1.83	0.44
1:B:4205:ARG:HG3	1:B:4312:GLN:HB3	1.99	0.44
1:A:2318:VAL:HG13	1:A:2344:LEU:HG	2.00	0.44
1:A:2557:LEU:HD21	1:A:2566:GLU:HB3	1.99	0.43
1:A:2632:LEU:HD22	1:A:2641:VAL:HG11	2.00	0.43
1:B:2082:LEU:HD12	1:B:2082:LEU:HA	1.84	0.43
1:A:1101:LEU:HB2	1:A:1197:LEU:HB2	1.99	0.43
1:A:1472:ARG:HD2	1:A:1930:LEU:HD13	2.01	0.43
1:A:4205:ARG:HG3	1:A:4312:GLN:HB3	1.99	0.43
1:B:988:LEU:HD12	1:B:997:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ILE:HD13	1:A:1272:LEU:HD21	2.00	0.43
1:B:2322:VAL:HG21	1:B:2360:ILE:HG12	2.00	0.43
1:A:2783:GLN:HG3	1:A:2832:GLN:HE22	1.84	0.43
1:A:2798:LEU:HD13	1:A:2829:THR:HG22	2.00	0.43
1:B:2798:LEU:HD13	1:B:2829:THR:HG22	2.01	0.43
1:B:3352:LEU:HD11	1:B:3416:SER:HB3	2.00	0.43
1:A:2853:VAL:HG11	1:A:2909:LEU:HD21	2.01	0.43
1:B:1515:LEU:HD11	1:B:2062:LEU:HD21	2.00	0.43
1:B:1090:ILE:HD13	1:B:1272:LEU:HD21	2.00	0.43
1:B:1472:ARG:HD2	1:B:1930:LEU:HD13	2.01	0.43
1:B:2713:THR:O	1:B:2716:THR:OG1	2.31	0.43
1:B:2783:GLN:HG3	1:B:2832:GLN:HE22	1.84	0.43
1:A:68:VAL:O	1:A:77:LEU:N	2.45	0.43
1:A:3846:LEU:HD13	1:A:3850:THR:HG21	2.01	0.43
1:A:3051:TYR:CD1	1:A:3052:MET:HG2	2.54	0.42
1:B:2632:LEU:HD22	1:B:2641:VAL:HG11	2.00	0.42
1:A:1803:ILE:HG22	1:A:1818:VAL:HG12	2.01	0.42
1:B:1298:MET:HE3	1:B:1298:MET:HB2	1.96	0.42
1:B:3147:HIS:HE1	1:B:3293:THR:O	2.01	0.42
1:B:3552:ILE:HG21	1:B:3617:LEU:HD12	2.01	0.42
1:A:1194:ARG:HA	1:A:1194:ARG:HD3	1.88	0.42
1:A:3352:LEU:HD11	1:A:3416:SER:HB3	2.00	0.42
1:B:140:LEU:O	1:B:194:VAL:N	2.44	0.42
1:B:2318:VAL:HG13	1:B:2344:LEU:HG	2.00	0.42
1:B:3051:TYR:CD1	1:B:3052:MET:HG2	2.54	0.42
1:B:2021:LEU:HD13	1:B:2584:LEU:HD21	2.01	0.42
1:B:2311:HIS:HE1	1:B:2355:ILE:HG23	1.84	0.42
1:A:1487:LEU:HD22	1:A:1968:LEU:HD11	2.02	0.42
1:A:2135:LEU:HD12	1:A:2135:LEU:HA	1.91	0.42
1:A:1515:LEU:HD11	1:A:2062:LEU:HD21	2.00	0.42
1:B:3146:ILE:HG13	1:B:3285:LEU:HD23	2.02	0.42
1:A:140:LEU:O	1:A:194:VAL:N	2.43	0.42
1:A:3146:ILE:HG13	1:A:3285:LEU:HD23	2.02	0.42
1:A:3552:ILE:HG21	1:A:3617:LEU:HD12	2.01	0.42
1:A:1083:LYS:HB2	1:A:1277:SER:HB2	2.02	0.42
1:A:1158:LEU:HD12	1:A:1184:LEU:HA	2.02	0.42
1:A:2034:ALA:O	1:A:2038:SER:OG	2.32	0.42
1:B:1487:LEU:HD22	1:B:1968:LEU:HD11	2.02	0.42
1:B:1803:ILE:HG22	1:B:1818:VAL:HG12	2.01	0.42
1:B:3701:LEU:HD13	1:B:3749:THR:HG23	2.01	0.42
1:A:988:LEU:HD12	1:A:997:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:PHE:HE2	1:A:1416:LEU:HA	1.85	0.42
1:B:1542:PRO:HB2	1:B:1759:PRO:HD3	2.02	0.42
1:B:3846:LEU:HD13	1:B:3850:THR:HG21	2.01	0.42
1:A:2311:HIS:HE1	1:A:2355:ILE:HG23	1.84	0.41
1:A:1415:PHE:HB3	1:A:1991:LEU:HD23	2.02	0.41
1:A:2021:LEU:HD13	1:A:2584:LEU:HD21	2.02	0.41
1:A:4211:THR:HG21	1:A:4221:LEU:HD23	2.02	0.41
1:A:4428:MET:HE2	1:A:4428:MET:HB2	1.84	0.41
1:B:135:VAL:HA	1:B:199:PRO:HA	2.02	0.41
1:B:1371:PHE:HE2	1:B:1416:LEU:HA	1.85	0.41
1:B:1433:ASN:HA	1:B:1436:LYS:HZ3	1.84	0.41
1:B:2795:SER:HB3	1:B:2834:PHE:HD1	1.85	0.41
1:B:4211:THR:HG21	1:B:4221:LEU:HD23	2.02	0.41
1:A:1542:PRO:HB2	1:A:1759:PRO:HD3	2.02	0.41
1:A:2082:LEU:HD12	1:A:2082:LEU:HA	1.84	0.41
1:A:2795:SER:HB3	1:A:2834:PHE:HD1	1.84	0.41
1:B:2853:VAL:HG11	1:B:2909:LEU:HD21	2.01	0.41
1:A:135:VAL:HA	1:A:199:PRO:HA	2.02	0.41
1:A:1943:LEU:HG	1:B:3114:THR:HG22	2.03	0.41
1:A:2166:ASP:OD2	1:A:2342:LYS:NZ	2.44	0.41
1:A:3318:ARG:HG2	1:A:3359:MET:SD	2.61	0.41
1:B:1083:LYS:HB2	1:B:1277:SER:HB2	2.02	0.41
1:B:2554:ASP:N	1:B:2554:ASP:OD1	2.53	0.41
1:A:2151:ILE:HD13	1:A:2151:ILE:HA	1.91	0.41
1:A:4167:HIS:HB3	1:A:4199:LEU:HD21	2.02	0.41
1:A:4377:PRO:HA	1:A:4380:ARG:HE	1.86	0.41
1:B:1443:CYS:O	1:B:1447:CYS:CB	2.69	0.41
1:B:3797:LEU:O	1:B:3801:LEU:CB	2.68	0.41
1:B:1148:PRO:HA	1:B:1151:GLU:HB3	2.02	0.41
1:B:4432:VAL:HG13	1:B:4466:VAL:HG12	2.03	0.41
1:B:4436:THR:HA	1:B:4439:LEU:HG	2.03	0.41
1:A:998:LEU:HB3	1:A:1328:LEU:HB3	2.02	0.41
1:A:1029:GLN:HG3	1:A:1033:ARG:HE	1.86	0.41
1:A:1916:LEU:HD23	1:B:3800:GLN:HE21	1.85	0.41
1:A:4238:LEU:HD13	1:A:4356:LEU:HD13	2.03	0.41
1:B:2655:LEU:HD23	1:B:2655:LEU:HA	1.93	0.41
1:B:2826:LEU:HD23	1:B:2826:LEU:HA	1.91	0.41
1:B:3445:ASP:HB3	1:B:3472:LEU:HD13	2.03	0.41
1:A:1011:THR:O	1:A:1049:HIS:ND1	2.54	0.41
1:A:2036:LEU:HD23	1:A:2071:LEU:HD13	2.03	0.41
1:A:3330:LEU:O	1:A:3334:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3701:LEU:HD13	1:A:3749:THR:HG23	2.01	0.41
1:B:998:LEU:HB3	1:B:1328:LEU:HB3	2.02	0.41
1:A:4357:ILE:HA	1:A:4360:MET:HG3	2.03	0.41
1:A:1148:PRO:HA	1:A:1151:GLU:HB3	2.02	0.40
1:A:3800:GLN:HE21	1:B:1916:LEU:HD23	1.85	0.40
1:A:1511:LEU:HD12	1:A:2105:MET:HB3	2.04	0.40
1:A:2554:ASP:OD1	1:A:2554:ASP:N	2.53	0.40
1:A:2702:LEU:HG	1:A:2703:ARG:NH1	2.37	0.40
1:A:3797:LEU:O	1:A:3801:LEU:CB	2.68	0.40
1:B:1014:PHE:CE1	1:B:1069:LEU:HD22	2.56	0.40
1:B:1415:PHE:HB3	1:B:1991:LEU:HD23	2.02	0.40
1:B:2702:LEU:HG	1:B:2703:ARG:NH1	2.37	0.40
1:A:1380:LYS:HE2	1:A:1834:ILE:HG23	2.03	0.40
1:A:3114:THR:HG22	1:B:1943:LEU:HG	2.03	0.40
1:A:3599:LEU:HD23	1:A:3599:LEU:HA	1.98	0.40
1:A:3807:LYS:HA	1:A:3847:PRO:HA	2.03	0.40
1:B:1194:ARG:HA	1:B:1194:ARG:HD3	1.88	0.40
1:B:1380:LYS:HE2	1:B:1834:ILE:HG23	2.03	0.40
1:B:3613:LEU:HD23	1:B:3613:LEU:HA	1.95	0.40
1:A:4436:THR:HA	1:A:4439:LEU:HG	2.03	0.40
1:B:1158:LEU:HD12	1:B:1184:LEU:HA	2.02	0.40
1:B:1357:LYS:HA	1:B:1360:LYS:HD2	2.03	0.40
1:B:2651:LEU:HD21	1:B:2711:SER:HA	2.04	0.40
1:B:3318:ARG:HG2	1:B:3359:MET:SD	2.60	0.40
1:B:1043:HIS:CE1	1:B:1815:ARG:HA	2.57	0.40
1:B:2373:LEU:HD23	1:B:2373:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2841/4896 (58%)	2786 (98%)	55 (2%)	0	100	100
1	B	2841/4896 (58%)	2787 (98%)	54 (2%)	0	100	100
All	All	5682/9792 (58%)	5573 (98%)	109 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2046/4236 (48%)	2043 (100%)	3 (0%)	93	98
1	B	2046/4236 (48%)	2043 (100%)	3 (0%)	93	98
All	All	4092/8472 (48%)	4086 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1775	ARG
1	A	2313	ARG
1	A	4429	LYS
1	B	1775	ARG
1	B	2313	ARG
1	B	4429	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1056	GLN
1	A	2311	HIS
1	A	2656	ASN
1	A	3147	HIS
1	B	1056	GLN
1	B	2311	HIS
1	B	2656	ASN

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Mol	Chain	Res	Type
1	B	3147	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.