



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:17 AM UTC

PDB ID : 4ILM / pdb_00004ilm
Title : CRISPR RNA Processing endoribonuclease
Authors : Shao, Y.; Li, H.
Deposited on : 2012-12-31
Resolution : 3.07 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

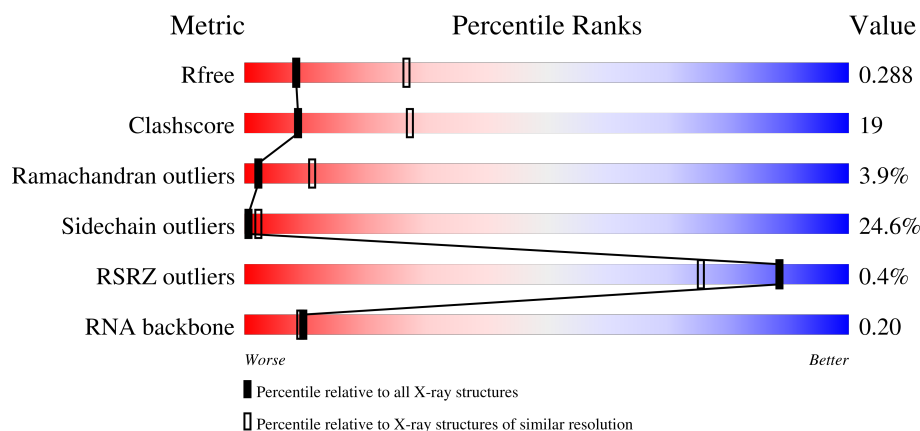
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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	289	
1	B	289	
1	D	289	
1	F	289	

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Mol	Chain	Length	Quality of chain
1	H	289	
1	J	289	
1	L	289	
1	N	289	
2	C	16	
2	E	16	
2	G	16	
2	I	16	
2	K	16	
2	M	16	
2	O	16	
2	R	16	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20435 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 CRISPR-associated endoribonuclease Cas6 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2223	1443	381	395	4			
1	B	281	Total	C	N	O	S	0	0	0
			2240	1452	385	399	4			
1	D	276	Total	C	N	O	S	0	0	0
			2205	1433	378	390	4			
1	F	278	Total	C	N	O	S	0	0	0
			2219	1440	380	395	4			
1	H	276	Total	C	N	O	S	0	0	0
			2205	1433	378	390	4			
1	J	283	Total	C	N	O	S	0	0	0
			2258	1462	387	405	4			
1	L	278	Total	C	N	O	S	0	0	0
			2223	1443	380	396	4			
1	N	274	Total	C	N	O	S	0	0	0
			2190	1425	375	386	4			

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	C	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	E	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	G	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	I	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	K	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			

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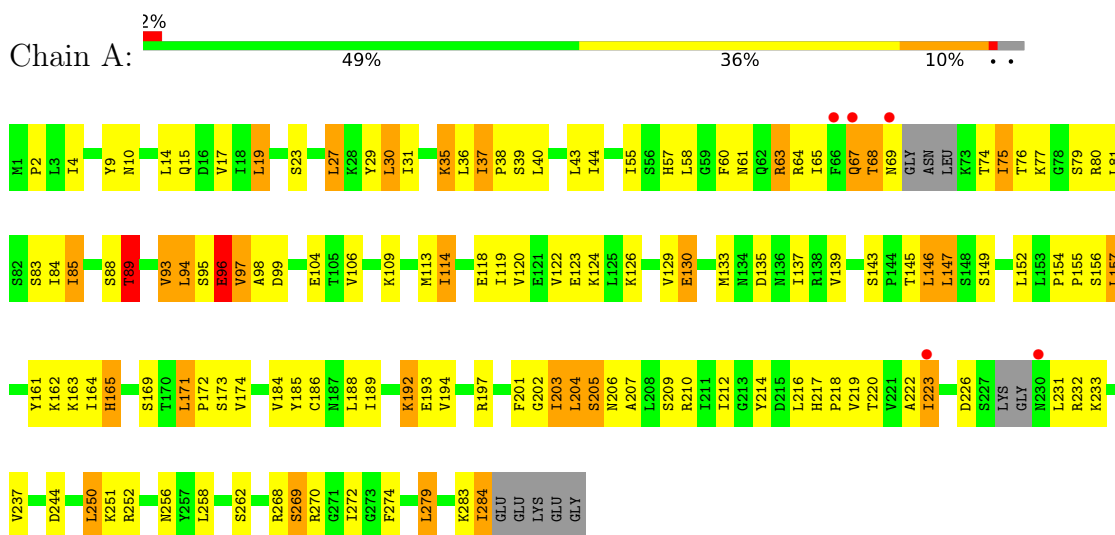
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			
2	O	16	Total	C	N	O	P	0	0	0
			334	152	59	108	15			

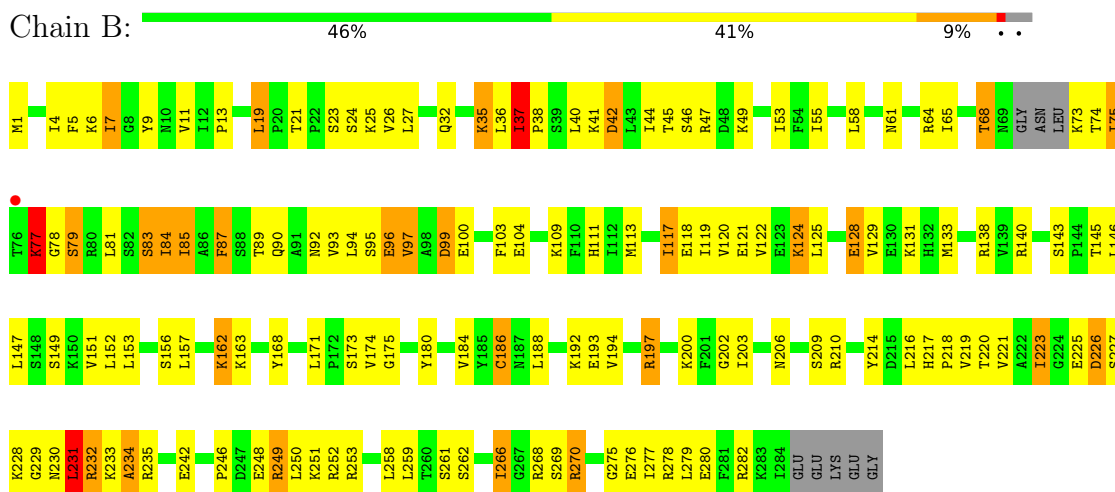
3 Residue-property plots

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: CRISPR-associated endoribonuclease Cas6 2

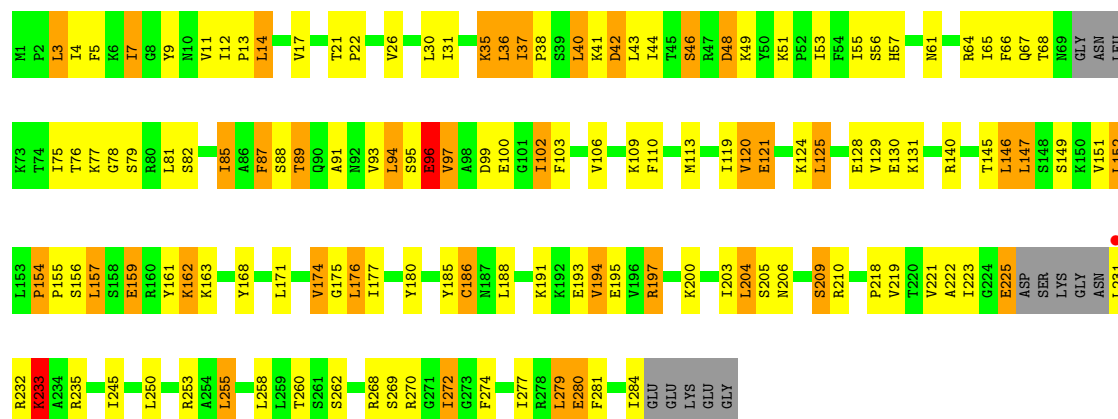


• Molecule 1: CRISPR-associated endoribonuclease Cas6 2



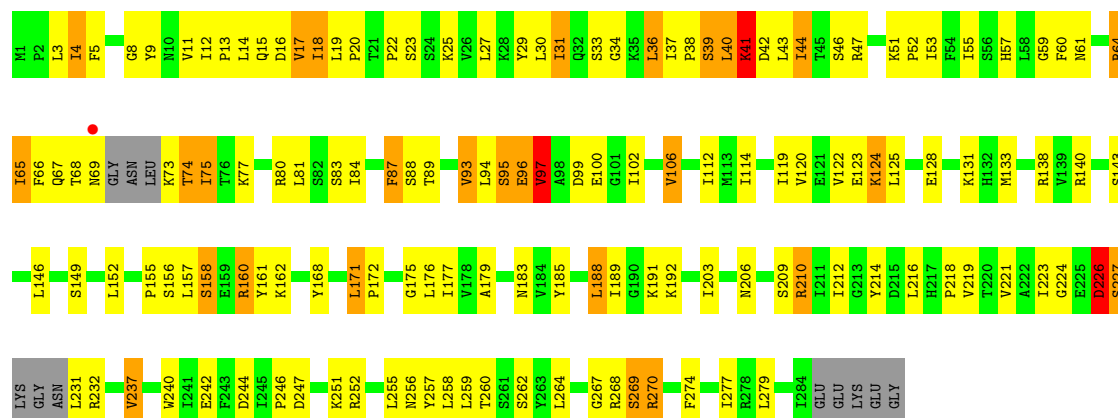
• Molecule 1: CRISPR-associated endoribonuclease Cas6 2





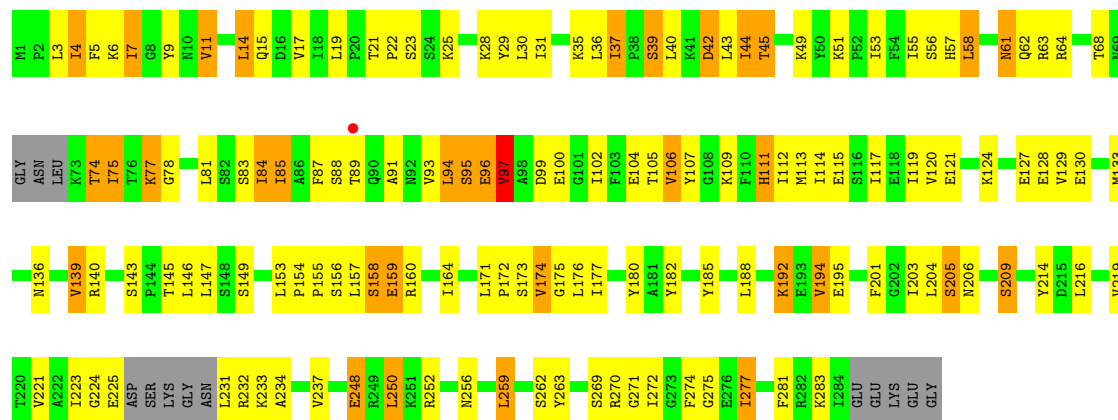
• Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain F: 46% 40% 9% . .



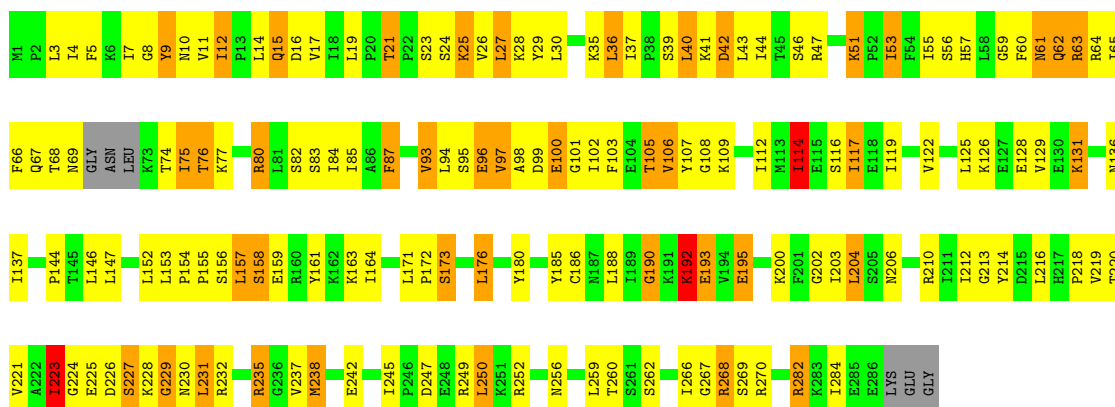
• Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain H: 45% 38% 11% .



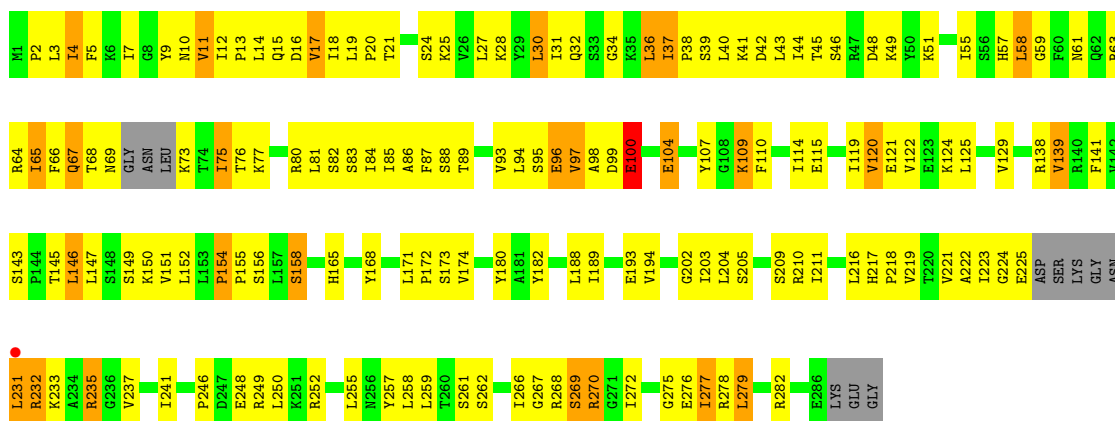
• Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain J: 43% 39% 15% . .



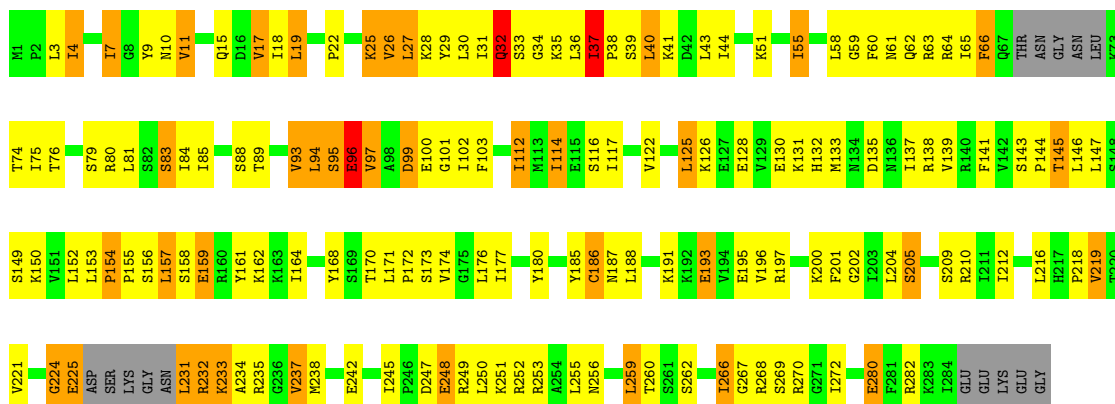
• Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain L: 41% 46% 9% .



• Molecule 1: CRISPR-associated endoribonuclease Cas6 2

Chain N: 40% 40% 13% . 5%

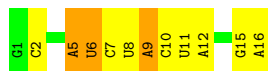


• Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')

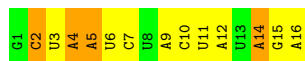
Chain R: 44% 44% 12%



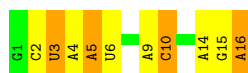
- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')



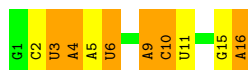
- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')



- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')



- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')

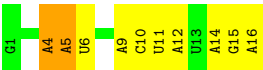


- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')

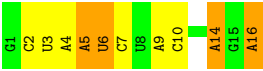


- Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')





● Molecule 2: RNA (5'-R(*GP*CP*UP*AP*AP*UP*CP*UP*AP*CP*UP*AP*UP*AP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.98Å 154.61Å 130.85Å 90.00° 93.64° 90.00°	Depositor
Resolution (Å)	35.00 – 3.07 35.00 – 3.07	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.00-3.07) 92.0 (35.00-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.233 , 0.284 0.237 , 0.288	Depositor DCC
R_{free} test set	2008 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20435	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.43	0/2264	0.91	2/3051 (0.1%)
1	B	0.45	0/2282	0.97	4/3075 (0.1%)
1	D	0.42	0/2246	0.92	6/3026 (0.2%)
1	F	0.45	0/2260	0.94	1/3045 (0.0%)
1	H	0.42	0/2246	0.95	4/3026 (0.1%)
1	J	0.42	0/2300	0.93	5/3099 (0.2%)
1	L	0.41	0/2264	0.89	3/3050 (0.1%)
1	N	0.41	0/2231	0.94	6/3005 (0.2%)
2	C	0.44	0/373	0.64	0/579
2	E	0.25	0/373	0.70	0/579
2	G	0.20	0/373	0.58	0/579
2	I	0.22	0/373	0.67	0/579
2	K	0.25	0/373	0.52	0/579
2	M	0.20	0/373	0.56	0/579
2	O	0.29	0/373	0.57	0/579
2	R	0.21	0/373	0.59	0/579
All	All	0.41	0/21077	0.89	31/29009 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LYS	N-CA-C	-7.74	103.80	113.55
1	B	37	ILE	CA-C-N	7.01	126.64	119.56
1	B	37	ILE	C-N-CA	7.01	126.64	119.56
1	B	35	LYS	N-CA-C	-6.91	104.85	113.55
1	A	60	PHE	N-CA-C	-6.73	99.33	110.17
1	N	224	GLY	CA-C-O	-6.60	116.02	121.76
1	N	154	PRO	CA-C-N	6.47	126.16	119.56
1	N	154	PRO	C-N-CA	6.47	126.16	119.56
1	J	106	VAL	N-CA-C	-6.36	104.42	113.07
1	D	154	PRO	CA-C-N	6.34	126.25	119.28
1	D	154	PRO	C-N-CA	6.34	126.25	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ILE	N-CA-C	6.29	116.88	107.51
1	N	232	ARG	CG-CD-NE	-6.21	98.33	112.00
1	J	229	GLY	N-CA-C	-6.09	98.74	113.18
1	J	245	ILE	CA-C-N	5.95	125.63	119.56
1	J	245	ILE	C-N-CA	5.95	125.63	119.56
1	N	245	ILE	CA-C-N	5.77	125.44	119.56
1	N	245	ILE	C-N-CA	5.77	125.44	119.56
1	H	35	LYS	N-CA-C	-5.73	106.33	113.55
1	J	114	ILE	N-CA-C	5.63	116.23	108.12
1	D	245	ILE	CA-C-N	5.53	125.20	119.56
1	D	245	ILE	C-N-CA	5.53	125.20	119.56
1	H	78	GLY	N-CA-C	-5.49	107.20	115.32
1	D	35	LYS	N-CA-C	-5.41	106.73	113.55
1	L	154	PRO	CA-C-N	5.37	125.69	119.47
1	L	154	PRO	C-N-CA	5.37	125.69	119.47
1	F	31	ILE	N-CA-C	-5.27	105.26	111.00
1	L	87	PHE	N-CA-C	5.18	116.17	108.60
1	H	248	GLU	N-CA-C	5.17	116.60	111.07
1	B	234	ALA	N-CA-C	5.09	117.29	109.95
1	H	7	ILE	N-CA-C	5.03	115.15	108.11

There are no chirality outliers.

There are no planarity outliers.

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	2223	0	2327	70	1
1	B	2240	0	2351	112	0
1	D	2205	0	2319	93	0
1	F	2219	0	2328	94	0
1	H	2205	0	2319	81	0
1	J	2258	0	2363	104	1
1	L	2223	0	2331	88	0
1	N	2190	0	2306	109	1
2	C	334	0	170	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	334	0	170	20	1
2	G	334	0	170	10	1
2	I	334	0	170	8	0
2	K	334	0	170	3	0
2	M	334	0	170	6	0
2	O	334	0	170	18	0
2	R	334	0	170	4	0
All	All	20435	0	20004	751	3

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 19.

All (751) 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:210:ARG:HH12	1:B:246:PRO:HG3	1.30	0.95
1:J:57:HIS:O	1:J:64:ARG:NH1	2.02	0.93
1:F:57:HIS:HB2	1:F:64:ARG:HG3	1.52	0.90
1:H:55:ILE:HG22	1:H:85:ILE:HG12	1.52	0.90
2:I:6:U:H3	2:I:16:A:H61	0.93	0.90
1:B:232:ARG:NH1	2:C:6:U:O4'	2.05	0.88
1:F:31:ILE:O	1:F:41:LYS:NZ	2.06	0.87
1:J:69:ASN:ND2	1:J:220:THR:O	2.08	0.87
2:I:6:U:H3	2:I:16:A:N6	1.74	0.85
1:F:13:PRO:HG3	1:F:75:ILE:HD11	1.59	0.84
1:N:232:ARG:NH2	2:O:7:C:C2	2.44	0.84
1:B:140:ARG:NH1	1:B:280:GLU:OE1	2.10	0.84
1:H:104:GLU:HG3	1:H:109:LYS:HG3	1.60	0.83
1:L:31:ILE:O	1:L:41:LYS:NZ	2.10	0.82
1:H:57:HIS:O	1:H:64:ARG:NH1	2.13	0.82
1:D:35:LYS:HD3	1:D:103:PHE:HD1	1.44	0.82
1:N:59:GLY:HA2	1:N:65:ILE:HG13	1.61	0.81
1:J:61:ASN:OD1	1:J:63:ARG:HG3	1.80	0.81
1:J:173:SER:HB2	1:J:206:ASN:HD21	1.43	0.81
1:D:233:LYS:NZ	2:E:6:U:H5'	1.94	0.81
1:N:133:MET:HE2	1:N:248:GLU:HG2	1.62	0.80
1:N:233:LYS:NZ	2:O:6:U:OP1	2.15	0.80
1:D:49:LYS:NZ	2:E:12:A:OP1	2.15	0.80
1:N:224:GLY:O	1:N:232:ARG:HG3	1.81	0.79
1:J:37:ILE:HG23	1:J:93:VAL:HG11	1.64	0.79
1:A:173:SER:HB3	1:A:206:ASN:HD21	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:232:ARG:NH2	2:O:6:U:O2	2.16	0.78
1:N:125:LEU:HB3	1:N:259:LEU:HD11	1.63	0.78
1:N:197:ARG:HH21	1:N:253:ARG:HH22	1.30	0.78
1:D:46:SER:OG	1:D:48:ASP:OD1	2.02	0.78
1:B:5:PHE:HD1	1:B:119:ILE:HD12	1.49	0.77
1:B:40:LEU:HD11	1:B:87:PHE:HE2	1.50	0.77
1:F:34:GLY:HA2	1:F:38:PRO:HB3	1.66	0.77
1:B:146:LEU:HB3	1:B:168:TYR:CE1	2.20	0.76
1:F:161:TYR:OH	1:J:249:ARG:NH2	2.19	0.76
1:B:223:ILE:HD11	1:B:232:ARG:NH2	2.02	0.75
1:B:5:PHE:HB2	1:B:87:PHE:HE1	1.50	0.75
1:J:224:GLY:HA2	1:J:232:ARG:HE	1.50	0.75
1:F:20:PRO:HB2	1:F:25:LYS:HD3	1.70	0.74
1:B:111:HIS:HE1	1:B:113:MET:HE2	1.53	0.74
1:L:223:ILE:HG22	1:L:224:GLY:H	1.53	0.73
1:J:105:THR:OG1	1:J:108:GLY:O	2.06	0.73
1:D:205:SER:O	1:D:209:SER:OG	2.03	0.73
1:A:204:LEU:HD23	1:A:250:LEU:HD11	1.70	0.73
1:A:212:ILE:O	1:B:235:ARG:NH1	2.21	0.73
1:D:233:LYS:HZ3	2:E:5:A:H4'	1.53	0.73
1:L:25:LYS:NZ	1:L:224:GLY:O	2.19	0.73
1:B:49:LYS:NZ	2:C:12:A:OP1	2.22	0.72
1:N:233:LYS:HE2	2:O:5:A:H5''	1.72	0.72
1:L:121:GLU:HG2	1:L:124:LYS:HD3	1.69	0.72
1:N:95:SER:O	1:N:97:VAL:N	2.21	0.72
1:J:268:ARG:NH2	2:K:14:A:N7	2.37	0.71
1:B:223:ILE:HG13	1:B:232:ARG:HG3	1.71	0.71
1:B:223:ILE:HD11	1:B:232:ARG:HH21	1.55	0.71
1:N:147:LEU:HD23	1:N:176:LEU:HB3	1.72	0.71
1:N:55:ILE:HD12	1:N:85:ILE:HD13	1.72	0.71
1:H:283:LYS:HB2	1:N:76:THR:HG21	1.73	0.70
1:B:5:PHE:HB2	1:B:87:PHE:CE1	2.25	0.70
1:J:128:GLU:HA	1:J:131:LYS:HE2	1.72	0.70
1:A:19:LEU:HG	1:A:75:ILE:HD11	1.74	0.70
1:L:120:VAL:HG23	1:L:124:LYS:HE2	1.73	0.70
1:N:152:LEU:HD21	1:N:202:GLY:HA3	1.74	0.70
1:F:244:ASP:OD1	1:F:251:LYS:NZ	2.25	0.70
1:N:126:LYS:HE3	1:N:256:ASN:HD21	1.57	0.69
1:H:39:SER:OG	1:H:96:GLU:OE2	2.10	0.69
1:A:67:GLN:O	1:A:69:ASN:N	2.25	0.69
1:L:57:HIS:O	1:L:64:ARG:NH1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:225:GLU:OE1	1:L:231:LEU:N	2.24	0.69
1:N:153:LEU:HD12	1:N:154:PRO:HD2	1.75	0.69
1:D:193:GLU:CD	1:F:160:ARG:HE	2.01	0.69
1:J:5:PHE:HB2	1:J:87:PHE:HE2	1.57	0.69
1:D:186:CYS:SG	1:D:194:VAL:HG21	2.33	0.68
1:B:232:ARG:HH22	1:B:234:ALA:HB2	1.58	0.68
1:L:262:SER:HB2	1:L:279:LEU:HD12	1.74	0.68
1:J:35:LYS:HB3	1:J:103:PHE:CE1	2.28	0.68
1:N:38:PRO:HA	1:N:41:LYS:HE2	1.75	0.68
1:D:233:LYS:NZ	2:E:5:A:H4'	2.07	0.68
1:J:5:PHE:HD1	1:J:119:ILE:HG12	1.57	0.68
1:N:141:PHE:CD1	1:N:145:THR:HG21	2.28	0.68
2:G:4:A:OP2	1:J:282:ARG:NH1	2.20	0.68
1:N:7:ILE:HG23	1:N:85:ILE:HG23	1.76	0.68
1:J:35:LYS:HB3	1:J:103:PHE:HE1	1.60	0.67
1:B:128:GLU:HA	1:B:131:LYS:HE2	1.75	0.67
1:N:235:ARG:HD2	2:O:4:A:H4'	1.75	0.67
1:A:201:PHE:O	1:A:205:SER:OG	2.11	0.67
1:N:141:PHE:HD1	1:N:145:THR:HG21	1.59	0.67
1:D:40:LEU:HG	1:D:43:LEU:HD11	1.76	0.66
1:D:233:LYS:HZ2	2:E:6:U:H5'	1.60	0.66
1:L:30:LEU:HD22	1:L:36:LEU:HD12	1.78	0.66
1:H:201:PHE:O	1:H:205:SER:OG	2.12	0.65
1:B:223:ILE:HD11	1:B:232:ARG:NE	2.12	0.65
1:N:232:ARG:NH2	2:O:16:A:H2	1.94	0.65
1:L:138:ARG:HH22	1:L:282:ARG:CZ	2.10	0.65
1:L:224:GLY:HA2	1:L:232:ARG:HD3	1.77	0.65
1:H:153:LEU:HD12	1:H:154:PRO:HD2	1.78	0.65
1:F:122:VAL:HG11	1:F:188:LEU:HD21	1.78	0.64
1:B:55:ILE:HG22	1:B:85:ILE:HG13	1.78	0.64
1:L:49:LYS:NZ	2:M:12:A:OP1	2.31	0.64
1:L:3:LEU:O	1:L:88:SER:OG	2.08	0.63
1:A:67:GLN:NE2	1:A:69:ASN:O	2.30	0.63
1:B:129:VAL:HG11	1:B:252:ARG:HG3	1.80	0.63
1:A:165:HIS:O	1:B:210:ARG:NH2	2.30	0.63
2:I:3:U:H4'	2:I:4:A:OP2	1.98	0.63
1:B:276:GLU:OE2	1:B:278:ARG:NH2	2.31	0.63
1:J:114:ILE:HD11	1:J:117:ILE:HD13	1.80	0.63
1:L:32:GLN:HG2	1:L:44:ILE:HD11	1.81	0.63
1:N:63:ARG:HE	1:N:66:PHE:HD2	1.44	0.62
1:N:138:ARG:HB3	1:N:280:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:172:PRO:HG3	1:N:237:VAL:HG21	1.78	0.62
1:B:232:ARG:HD3	2:C:6:U:O2	1.99	0.62
1:H:23:SER:HB2	1:H:58:LEU:HD22	1.81	0.62
1:H:159:GLU:OE1	1:H:160:ARG:N	2.30	0.62
1:B:13:PRO:HG2	1:B:78:GLY:HA2	1.80	0.62
1:F:175:GLY:HA3	1:F:206:ASN:HB2	1.81	0.62
1:J:40:LEU:HD23	1:J:87:PHE:HD1	1.64	0.62
1:D:31:ILE:O	1:D:41:LYS:HE2	2.00	0.62
1:A:130:GLU:OE2	1:A:252:ARG:NH2	2.31	0.62
1:H:102:ILE:HG12	1:H:111:HIS:HB3	1.80	0.62
1:D:30:LEU:HD13	1:D:36:LEU:HD21	1.82	0.62
1:H:225:GLU:H	1:H:231:LEU:HA	1.65	0.62
1:N:34:GLY:HA2	1:N:41:LYS:HZ1	1.64	0.62
1:B:223:ILE:HD11	1:B:232:ARG:CZ	2.30	0.62
1:D:89:THR:HG23	1:D:91:ALA:H	1.64	0.62
1:B:37:ILE:HG12	1:B:96:GLU:HG3	1.81	0.61
1:D:128:GLU:HA	1:D:131:LYS:HZ3	1.65	0.61
1:J:5:PHE:HB2	1:J:87:PHE:CE2	2.34	0.61
1:A:268:ARG:NH2	2:R:15:G:N7	2.47	0.61
1:F:5:PHE:HB2	1:F:87:PHE:HE2	1.65	0.61
1:F:120:VAL:HG23	1:F:124:LYS:HE2	1.83	0.61
1:A:9:TYR:HD2	1:A:27:LEU:HD11	1.66	0.61
1:L:125:LEU:HD23	1:L:259:LEU:HB3	1.83	0.61
1:N:232:ARG:CZ	2:O:16:A:H2	2.14	0.61
1:L:34:GLY:HA2	1:L:41:LYS:HZ1	1.65	0.61
1:B:138:ARG:NH2	1:B:280:GLU:OE2	2.31	0.61
1:F:214:TYR:CE2	1:J:218:PRO:HG3	2.34	0.61
1:L:2:PRO:HG2	1:L:122:VAL:HG21	1.81	0.61
1:A:152:LEU:HD21	1:A:202:GLY:HA3	1.82	0.60
1:F:43:LEU:HD13	1:F:53:ILE:HG12	1.82	0.60
1:N:122:VAL:HG21	1:N:188:LEU:HD21	1.83	0.60
1:B:232:ARG:NH2	1:B:234:ALA:HB2	2.15	0.60
1:D:232:ARG:NH1	2:E:7:C:O2	2.34	0.60
1:H:36:LEU:HG	1:H:37:ILE:HG22	1.83	0.60
1:F:67:GLN:O	1:F:69:ASN:N	2.35	0.60
1:F:226:ASP:N	1:F:226:ASP:OD1	2.35	0.60
1:H:25:LYS:O	1:H:28:LYS:HB3	2.02	0.60
1:J:12:ILE:HG12	1:J:80:ARG:HD2	1.83	0.60
1:B:7:ILE:HD12	1:B:117:ILE:HG12	1.83	0.59
1:B:233:LYS:O	2:C:5:A:H4'	2.01	0.59
1:L:261:SER:HB3	1:L:266:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:GLU:CD	1:J:230:ASN:H	2.10	0.59
1:D:14:LEU:HD22	1:D:102:ILE:HD11	1.85	0.59
1:H:74:THR:OG1	1:H:75:ILE:N	2.36	0.59
1:B:122:VAL:HG11	1:B:188:LEU:HD21	1.84	0.59
1:N:225:GLU:OE2	1:N:231:LEU:N	2.36	0.59
1:B:197:ARG:NH1	1:J:159:GLU:OE2	2.35	0.59
1:H:29:TYR:CD2	1:H:105:THR:HG23	2.38	0.58
1:D:258:LEU:HB3	1:D:279:LEU:HD11	1.85	0.58
1:J:29:TYR:CD2	1:J:105:THR:HG22	2.38	0.58
1:L:172:PRO:HG3	1:L:237:VAL:HG11	1.85	0.58
1:B:223:ILE:HD11	1:B:232:ARG:HE	1.68	0.58
1:A:29:TYR:CE1	1:A:106:VAL:HG13	2.38	0.58
1:L:27:LEU:HD13	1:L:85:ILE:HD11	1.86	0.58
1:L:28:LYS:O	1:L:32:GLN:N	2.36	0.58
2:O:7:C:H42	2:O:14:A:H61	1.50	0.58
1:B:92:ASN:ND2	1:B:95:SER:HB3	2.18	0.58
1:F:5:PHE:HB2	1:F:87:PHE:CE2	2.39	0.58
2:G:4:A:N6	1:J:136:ASN:OD1	2.37	0.58
1:A:93:VAL:O	1:A:95:SER:N	2.36	0.58
1:J:43:LEU:O	1:J:51:LYS:NZ	2.34	0.58
1:J:146:LEU:HB2	1:J:268:ARG:O	2.03	0.58
1:F:185:TYR:HD1	1:F:260:THR:HG21	1.69	0.57
1:H:175:GLY:H	1:H:206:ASN:HB3	1.69	0.57
1:N:242:GLU:OE1	1:N:282:ARG:NH2	2.37	0.57
1:F:55:ILE:O	1:F:55:ILE:HG13	2.03	0.57
1:A:57:HIS:O	1:A:64:ARG:NH1	2.38	0.57
1:F:30:LEU:HD22	1:F:36:LEU:HD23	1.86	0.57
1:H:111:HIS:HB2	1:H:113:MET:HE1	1.85	0.57
1:N:219:VAL:HG11	1:N:238:MET:HE3	1.87	0.57
1:H:6:LYS:HE3	1:H:84:ILE:CG2	2.35	0.57
1:N:93:VAL:O	1:N:95:SER:N	2.38	0.57
1:F:224:GLY:HA3	1:F:232:ARG:NH2	2.20	0.57
1:N:27:LEU:HD13	1:N:30:LEU:HD21	1.86	0.57
1:B:5:PHE:CD1	1:B:119:ILE:HD12	2.35	0.57
1:J:129:VAL:HG11	1:J:252:ARG:HG3	1.85	0.57
1:L:210:ARG:HH11	1:L:246:PRO:HG3	1.70	0.57
1:F:268:ARG:NH1	2:G:14:A:N7	2.52	0.56
1:N:170:THR:HA	1:N:237:VAL:HG22	1.87	0.56
1:A:233:LYS:HG3	2:R:6:U:H5'	1.86	0.56
1:H:120:VAL:HG21	1:H:263:TYR:HE2	1.70	0.56
1:L:19:LEU:HD21	1:L:75:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:ILE:HG22	1:N:88:SER:HB2	1.87	0.56
1:N:132:HIS:ND1	1:N:135:ASP:OD1	2.37	0.56
1:B:266:ILE:HD12	1:B:277:ILE:HD13	1.87	0.56
1:D:40:LEU:HD23	1:D:44:ILE:HD11	1.86	0.56
1:F:146:LEU:HB2	1:F:268:ARG:O	2.06	0.56
1:J:37:ILE:HD11	1:J:97:VAL:HA	1.87	0.56
1:N:37:ILE:HG23	1:N:96:GLU:HG3	1.86	0.56
1:A:218:PRO:HG3	1:B:214:TYR:CE2	2.40	0.56
1:D:38:PRO:C	1:D:40:LEU:H	2.13	0.56
1:J:161:TYR:HD2	1:J:164:ILE:HD12	1.71	0.56
1:N:232:ARG:NE	2:O:16:A:H2	2.03	0.56
1:A:214:TYR:CE2	1:B:218:PRO:HG3	2.40	0.56
2:G:4:A:N7	1:J:136:ASN:ND2	2.48	0.55
1:N:15:GLN:HE21	1:N:17:VAL:HG13	1.72	0.55
1:A:104:GLU:OE1	1:A:104:GLU:N	2.38	0.55
1:F:20:PRO:HG2	1:F:25:LYS:HB2	1.87	0.55
1:J:5:PHE:CD1	1:J:119:ILE:HG12	2.41	0.55
1:H:172:PRO:HG3	1:H:237:VAL:HG11	1.88	0.55
1:L:145:THR:HG23	1:L:275:GLY:HA2	1.88	0.55
1:F:59:GLY:HA2	1:F:65:ILE:HG13	1.88	0.55
1:B:19:LEU:HD11	1:B:75:ILE:HG22	1.89	0.55
1:F:75:ILE:HD13	1:F:81:LEU:HD11	1.87	0.55
1:D:140:ARG:NH1	1:D:280:GLU:OE2	2.40	0.55
1:D:185:TYR:HD2	1:D:260:THR:HG21	1.72	0.55
1:F:15:GLN:O	1:F:17:VAL:HG12	2.07	0.55
1:D:268:ARG:NH1	2:E:14:A:N7	2.54	0.55
1:L:37:ILE:HB	1:L:40:LEU:HD13	1.88	0.55
1:D:38:PRO:O	1:D:41:LYS:HG2	2.07	0.55
2:O:16:A:H8	2:O:16:A:OP2	1.90	0.55
1:B:175:GLY:H	1:B:206:ASN:HB3	1.72	0.55
1:D:17:VAL:O	1:D:75:ILE:HG22	2.07	0.55
1:D:121:GLU:HG3	1:D:124:LYS:HB2	1.88	0.55
1:J:67:GLN:O	1:J:69:ASN:N	2.40	0.55
1:H:256:ASN:HA	1:H:259:LEU:HD12	1.89	0.54
1:L:7:ILE:HD13	1:L:9:TYR:CZ	2.42	0.54
1:B:220:THR:HG22	1:B:235:ARG:HG3	1.88	0.54
1:J:8:GLY:HA2	1:J:84:ILE:HD13	1.89	0.54
1:B:146:LEU:HB2	1:B:268:ARG:O	2.07	0.54
1:F:16:ASP:H	1:F:77:LYS:NZ	2.05	0.54
1:N:7:ILE:HB	1:N:117:ILE:HD13	1.89	0.54
1:N:27:LEU:HB3	1:N:55:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD21	1:B:202:GLY:HA3	1.90	0.54
1:B:225:GLU:O	1:B:226:ASP:HB2	2.07	0.54
1:N:232:ARG:NH2	2:O:16:A:C2	2.74	0.54
1:F:218:PRO:HG3	1:J:214:TYR:CE2	2.43	0.54
1:F:246:PRO:HB2	1:J:164:ILE:HG23	1.88	0.54
1:A:192:LYS:O	1:A:194:VAL:HG13	2.07	0.54
1:D:51:LYS:HG3	1:D:53:ILE:HG22	1.89	0.54
1:D:175:GLY:H	1:D:206:ASN:HB3	1.72	0.54
1:F:73:LYS:HG3	1:F:74:THR:H	1.72	0.54
1:N:146:LEU:HB3	1:N:168:TYR:CE1	2.43	0.54
1:B:40:LEU:HD11	1:B:87:PHE:CE2	2.39	0.54
1:H:17:VAL:O	1:H:75:ILE:HG23	2.07	0.54
1:B:47:ARG:HH21	2:C:11:U:H5	1.55	0.54
1:D:162:LYS:HD2	1:D:163:LYS:N	2.23	0.54
1:F:12:ILE:HG22	1:F:80:ARG:HA	1.89	0.54
1:L:4:ILE:HD11	1:L:188:LEU:HD21	1.88	0.54
1:L:270:ARG:NH2	2:M:15:G:OP1	2.36	0.54
1:N:22:PRO:HD2	1:N:25:LYS:HG2	1.89	0.54
1:N:232:ARG:NH1	2:O:7:C:H1'	2.23	0.54
1:B:232:ARG:NH1	1:B:233:LYS:H	2.05	0.53
1:L:147:LEU:HD22	1:L:180:TYR:CD2	2.43	0.53
1:D:48:ASP:OD1	1:D:48:ASP:N	2.37	0.53
1:D:129:VAL:HG22	1:D:255:LEU:HB3	1.90	0.53
1:D:197:ARG:NH1	1:D:253:ARG:HH12	2.07	0.53
1:J:59:GLY:HA2	1:J:65:ILE:HG12	1.89	0.53
1:N:38:PRO:O	1:N:41:LYS:HG2	2.09	0.53
1:B:37:ILE:HG23	1:B:96:GLU:CD	2.33	0.53
1:F:36:LEU:HG	1:F:37:ILE:HD12	1.91	0.53
1:H:49:LYS:NZ	2:I:11:U:O3'	2.37	0.53
1:J:232:ARG:HD2	2:K:7:C:H1'	1.91	0.53
1:L:7:ILE:HD11	1:L:85:ILE:HB	1.91	0.53
1:L:20:PRO:HB3	1:L:107:TYR:CE1	2.43	0.53
1:D:272:ILE:HG21	2:E:16:A:H3'	1.91	0.53
1:F:3:LEU:O	1:F:88:SER:OG	2.25	0.53
1:F:227:SER:HA	1:F:231:LEU:N	2.23	0.53
1:F:257:TYR:O	1:F:260:THR:OG1	2.18	0.53
1:F:52:PRO:C	1:F:53:ILE:HG13	2.34	0.53
1:N:172:PRO:HD2	1:N:216:LEU:HD13	1.91	0.53
1:A:126:LYS:O	1:A:129:VAL:HB	2.07	0.53
1:H:121:GLU:HG2	1:H:124:LYS:HB2	1.91	0.53
1:D:51:LYS:HE2	2:E:15:G:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HE	2:R:7:C:H1'	1.74	0.52
1:B:104:GLU:OE1	1:B:109:LYS:HG2	2.09	0.52
1:L:38:PRO:HA	1:L:41:LYS:HE2	1.90	0.52
1:N:32:GLN:O	1:N:32:GLN:NE2	2.42	0.52
1:D:191:LYS:HE3	1:F:155:PRO:O	2.08	0.52
1:L:88:SER:O	1:L:89:THR:OG1	2.23	0.52
1:A:146:LEU:HB2	1:A:268:ARG:O	2.10	0.52
1:J:40:LEU:HD23	1:J:87:PHE:CD1	2.43	0.52
1:B:261:SER:HB3	1:B:266:ILE:HG13	1.92	0.52
1:J:101:GLY:N	1:J:103:PHE:HE2	2.08	0.52
1:N:99:ASP:O	1:N:100:GLU:HG3	2.10	0.52
1:N:247:ASP:HB3	1:N:250:LEU:HB2	1.90	0.52
1:A:30:LEU:HB3	1:A:36:LEU:HB2	1.90	0.52
1:A:93:VAL:O	1:A:96:GLU:HG2	2.09	0.52
1:J:172:PRO:HG3	1:J:237:VAL:HG11	1.92	0.52
1:N:100:GLU:OE2	1:N:114:ILE:HD12	2.10	0.52
1:N:248:GLU:CD	1:N:252:ARG:HH22	2.18	0.52
1:H:221:VAL:HG21	1:H:274:PHE:CZ	2.46	0.51
1:N:133:MET:HE1	1:N:251:LYS:HB3	1.92	0.51
1:A:126:LYS:HZ2	1:A:256:ASN:HD21	1.58	0.51
1:H:51:LYS:NZ	2:I:15:G:O3'	2.42	0.51
1:H:56:SER:OG	1:H:64:ARG:NH1	2.42	0.51
1:F:38:PRO:C	1:F:40:LEU:H	2.17	0.51
1:N:112:ILE:HD12	1:N:112:ILE:H	1.75	0.51
1:J:173:SER:HB2	1:J:206:ASN:ND2	2.19	0.51
1:L:58:LEU:HA	1:L:82:SER:O	2.11	0.51
1:F:16:ASP:H	1:F:77:LYS:HZ3	1.58	0.51
1:F:93:VAL:O	1:F:95:SER:N	2.44	0.51
1:F:172:PRO:HG3	1:F:237:VAL:HG11	1.93	0.51
1:B:186:CYS:SG	1:B:194:VAL:HG21	2.51	0.51
2:E:15:G:H2'	2:E:16:A:C8	2.46	0.51
1:J:56:SER:OG	1:J:64:ARG:NH1	2.43	0.51
1:N:31:ILE:C	1:N:33:SER:H	2.18	0.51
1:A:2:PRO:HD2	1:A:123:GLU:OE2	2.11	0.51
1:N:186:CYS:SG	1:N:187:ASN:N	2.83	0.51
1:F:123:GLU:OE1	1:F:123:GLU:N	2.42	0.51
1:H:7:ILE:HD11	1:H:9:TYR:CE1	2.46	0.51
1:H:37:ILE:HG12	1:H:40:LEU:HG	1.93	0.51
1:J:93:VAL:HG12	1:J:96:GLU:HB2	1.93	0.51
1:N:64:ARG:HH12	1:N:83:SER:HA	1.76	0.51
1:N:197:ARG:HH12	1:N:200:LYS:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:VAL:O	1:D:177:ILE:HG12	2.11	0.50
1:J:17:VAL:H	1:J:77:LYS:HB2	1.75	0.50
1:N:31:ILE:O	1:N:41:LYS:NZ	2.31	0.50
1:N:144:PRO:HG3	1:N:238:MET:HE2	1.92	0.50
1:D:233:LYS:HZ1	2:E:6:U:P	2.33	0.50
1:N:159:GLU:HA	1:N:162:LYS:HG2	1.92	0.50
1:A:135:ASP:O	1:A:251:LYS:NZ	2.44	0.50
1:J:152:LEU:HG	1:J:176:LEU:HD22	1.92	0.50
1:D:154:PRO:HB2	1:D:157:LEU:HD13	1.94	0.50
1:L:38:PRO:C	1:L:40:LEU:H	2.20	0.50
1:D:218:PRO:HB2	1:D:235:ARG:HH21	1.76	0.50
1:F:155:PRO:O	1:F:158:SER:HB3	2.12	0.50
1:J:51:LYS:HD3	1:J:53:ILE:HD11	1.93	0.50
1:L:155:PRO:O	1:L:158:SER:OG	2.27	0.50
1:N:256:ASN:O	1:N:260:THR:HG23	2.12	0.49
1:D:55:ILE:HG22	1:D:85:ILE:HG22	1.94	0.49
1:F:179:ALA:O	1:F:183:ASN:ND2	2.40	0.49
1:J:185:TYR:O	1:J:188:LEU:HB3	2.12	0.49
1:L:172:PRO:HD2	1:L:216:LEU:HD13	1.93	0.49
1:N:201:PHE:O	1:N:205:SER:OG	2.30	0.49
1:A:122:VAL:HG11	1:A:188:LEU:HD21	1.93	0.49
1:N:95:SER:C	1:N:96:GLU:HG2	2.36	0.49
1:B:35:LYS:NZ	1:B:104:GLU:O	2.45	0.49
1:D:49:LYS:HG2	2:E:14:A:H4'	1.95	0.49
1:H:39:SER:HG	1:H:96:GLU:CD	2.20	0.49
1:L:17:VAL:HG13	1:L:75:ILE:HD11	1.95	0.49
1:F:4:ILE:HD13	1:F:264:LEU:HD21	1.95	0.49
1:F:93:VAL:O	1:F:96:GLU:HG2	2.13	0.49
1:B:145:THR:HG23	1:B:275:GLY:HA2	1.94	0.49
1:F:43:LEU:HB2	1:F:53:ILE:HD11	1.95	0.49
1:N:61:ASN:C	1:N:63:ARG:H	2.20	0.49
1:A:135:ASP:OD1	1:A:283:LYS:NZ	2.45	0.49
1:B:128:GLU:O	1:B:131:LYS:HG2	2.12	0.49
1:D:35:LYS:HD3	1:D:103:PHE:CD1	2.35	0.49
1:F:30:LEU:HD21	1:F:36:LEU:H	1.77	0.49
1:H:234:ALA:HB2	2:I:6:U:C5	2.48	0.49
1:J:214:TYR:HB2	1:J:216:LEU:HD22	1.94	0.49
1:L:225:GLU:OE2	1:L:231:LEU:HD23	2.12	0.49
1:A:35:LYS:HE2	1:A:104:GLU:O	2.12	0.49
1:H:30:LEU:HB3	1:H:36:LEU:HB3	1.94	0.49
1:H:145:THR:HG23	1:H:275:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:TYR:HD1	1:J:260:THR:HG21	1.77	0.48
1:H:94:LEU:HD12	1:H:94:LEU:H	1.78	0.48
1:J:105:THR:HB	1:J:107:TYR:H	1.78	0.48
1:J:152:LEU:HD21	1:J:202:GLY:HA3	1.95	0.48
1:A:15:GLN:NE2	1:A:109:LYS:H	2.10	0.48
1:A:19:LEU:CG	1:A:75:ILE:HD11	2.41	0.48
1:D:5:PHE:HB2	1:D:87:PHE:CE1	2.48	0.48
1:J:9:TYR:OH	1:J:36:LEU:HD13	2.14	0.48
1:J:100:GLU:HA	1:J:112:ILE:HD11	1.95	0.48
1:L:37:ILE:CG2	1:L:96:GLU:HB3	2.43	0.48
1:B:268:ARG:HG2	2:C:15:G:OP2	2.13	0.48
1:D:3:LEU:O	1:D:88:SER:OG	2.24	0.48
1:H:61:ASN:HB3	1:H:62:GLN:OE1	2.14	0.48
1:N:225:GLU:HG2	1:N:231:LEU:HA	1.94	0.48
1:N:234:ALA:HB2	2:O:6:U:C5	2.49	0.48
1:A:173:SER:HB3	1:A:206:ASN:ND2	2.24	0.48
1:B:206:ASN:HA	1:B:209:SER:OG	2.13	0.48
1:B:232:ARG:HH22	1:B:234:ALA:CB	2.24	0.48
1:L:65:ILE:O	1:L:67:GLN:NE2	2.47	0.48
1:B:93:VAL:O	1:B:97:VAL:HG23	2.14	0.48
1:B:175:GLY:N	1:B:206:ASN:HB3	2.29	0.48
1:B:223:ILE:CD1	1:B:232:ARG:HH21	2.26	0.48
1:B:232:ARG:CD	2:C:6:U:O2	2.62	0.48
1:D:38:PRO:HD2	1:D:96:GLU:OE1	2.14	0.48
1:D:185:TYR:CD2	1:D:260:THR:HG21	2.49	0.48
1:A:223:ILE:HD12	1:A:274:PHE:CZ	2.48	0.47
1:L:272:ILE:HG21	2:M:16:A:H3'	1.95	0.47
1:D:49:LYS:HZ1	2:E:12:A:P	2.33	0.47
1:H:129:VAL:HG11	1:H:252:ARG:HG3	1.96	0.47
1:J:122:VAL:O	1:J:125:LEU:HG	2.14	0.47
1:L:98:ALA:O	1:L:100:GLU:HB3	2.14	0.47
1:N:9:TYR:HE2	1:N:114:ILE:HG22	1.79	0.47
1:N:31:ILE:CD1	1:N:36:LEU:HB3	2.44	0.47
1:D:221:VAL:O	1:D:233:LYS:HA	2.13	0.47
1:F:11:VAL:HG12	1:F:112:ILE:HD12	1.96	0.47
1:F:51:LYS:HB2	1:F:53:ILE:HD12	1.96	0.47
1:J:212:ILE:HG13	1:J:242:GLU:O	2.14	0.47
1:L:55:ILE:O	1:L:55:ILE:HG13	2.13	0.47
1:L:152:LEU:HD21	1:L:202:GLY:HA3	1.96	0.47
2:O:7:C:N4	2:O:14:A:H61	2.11	0.47
1:A:164:ILE:HD11	1:B:246:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:HG23	1:B:96:GLU:HG3	1.97	0.47
1:F:29:TYR:CE2	1:F:106:VAL:HG13	2.50	0.47
1:J:180:TYR:CE1	1:J:267:GLY:HA2	2.49	0.47
1:L:11:VAL:HG13	1:L:81:LEU:HB2	1.97	0.47
1:L:223:ILE:HD12	1:L:223:ILE:HG23	1.52	0.47
1:A:135:ASP:OD2	1:A:283:LYS:NZ	2.47	0.47
2:C:6:U:H1'	2:C:7:C:C6	2.50	0.47
1:L:5:PHE:O	1:L:86:ALA:HA	2.14	0.47
1:L:69:ASN:HB3	1:L:73:LYS:NZ	2.29	0.47
1:N:180:TYR:CD2	1:N:267:GLY:HA2	2.49	0.47
1:B:210:ARG:HB2	1:B:210:ARG:NH1	2.29	0.47
1:D:31:ILE:HG12	1:D:40:LEU:HD22	1.96	0.47
1:H:14:LEU:HG	1:H:109:LYS:HD3	1.97	0.47
1:H:224:GLY:O	1:H:232:ARG:N	2.47	0.47
1:J:16:ASP:OD1	1:J:77:LYS:HD2	2.14	0.47
1:L:59:GLY:O	1:L:82:SER:HB3	2.14	0.47
1:A:17:VAL:O	1:A:75:ILE:HD12	2.15	0.47
1:D:40:LEU:HG	1:D:43:LEU:HD21	1.96	0.47
1:F:64:ARG:HA	1:F:64:ARG:HD3	1.58	0.47
1:F:221:VAL:HG21	1:F:274:PHE:CE2	2.50	0.47
1:H:89:THR:HG23	1:H:91:ALA:H	1.79	0.47
1:H:206:ASN:HA	1:H:209:SER:OG	2.14	0.47
1:J:41:LYS:HG2	1:J:42:ASP:N	2.30	0.47
1:J:212:ILE:HD11	1:J:242:GLU:CG	2.45	0.47
1:N:25:LYS:O	1:N:29:TYR:N	2.44	0.47
1:N:103:PHE:CG	1:N:112:ILE:HD11	2.50	0.47
1:A:15:GLN:OE1	1:A:15:GLN:N	2.48	0.47
1:B:197:ARG:HD2	1:J:159:GLU:O	2.14	0.47
1:D:55:ILE:HA	1:D:85:ILE:HG22	1.97	0.47
1:J:128:GLU:O	1:J:131:LYS:HG2	2.15	0.47
1:J:225:GLU:OE2	1:J:226:ASP:N	2.48	0.47
1:B:96:GLU:H	1:B:96:GLU:HG2	1.56	0.47
1:H:214:TYR:HB2	1:H:216:LEU:HD22	1.97	0.47
1:J:76:THR:HB	1:J:77:LYS:H	1.55	0.47
1:L:16:ASP:OD1	1:L:77:LYS:N	2.48	0.47
1:N:38:PRO:C	1:N:40:LEU:H	2.21	0.47
1:B:23:SER:O	1:B:26:VAL:HG22	2.16	0.46
1:L:211:ILE:HD12	1:L:241:ILE:HD11	1.95	0.46
1:F:172:PRO:HB3	1:F:177:ILE:HD11	1.97	0.46
1:J:153:LEU:HD12	1:J:154:PRO:HD2	1.98	0.46
1:J:200:LYS:O	1:J:204:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:TYR:HB2	1:F:216:LEU:HD22	1.95	0.46
1:H:43:LEU:HD11	1:H:89:THR:OG1	2.16	0.46
1:J:36:LEU:HG	1:J:37:ILE:N	2.28	0.46
1:L:141:PHE:HA	1:L:277:ILE:HD12	1.97	0.46
1:B:7:ILE:HG12	1:B:9:TYR:CE2	2.51	0.46
1:B:74:THR:OG1	1:B:75:ILE:N	2.49	0.46
1:F:18:ILE:H	1:F:18:ILE:HG13	1.36	0.46
1:B:87:PHE:HZ	1:B:93:VAL:HG11	1.80	0.46
1:F:267:GLY:O	1:F:270:ARG:NH1	2.40	0.46
1:N:101:GLY:O	1:N:112:ILE:HD12	2.15	0.46
1:N:128:GLU:O	1:N:131:LYS:HG2	2.16	0.46
1:N:218:PRO:HB2	1:N:235:ARG:HH22	1.81	0.46
1:B:42:ASP:HA	1:B:45:THR:HG22	1.98	0.46
1:D:31:ILE:HG21	1:D:40:LEU:HB3	1.98	0.46
1:F:185:TYR:CD1	1:F:260:THR:HG21	2.50	0.46
1:H:15:GLN:O	1:H:77:LYS:HB2	2.16	0.46
1:B:111:HIS:CE1	1:B:113:MET:HE2	2.42	0.46
1:D:200:LYS:O	1:D:204:LEU:HB2	2.16	0.46
1:H:6:LYS:HE3	1:H:84:ILE:HG21	1.97	0.46
1:H:62:GLN:NE2	1:H:63:ARG:HG3	2.30	0.46
1:D:43:LEU:HD12	1:D:44:ILE:HG12	1.98	0.46
1:F:43:LEU:HD12	1:F:44:ILE:HG12	1.97	0.46
1:F:133:MET:HE1	1:F:252:ARG:HA	1.97	0.46
1:H:185:TYR:O	1:H:188:LEU:HB3	2.16	0.46
1:J:93:VAL:O	1:J:95:SER:N	2.49	0.46
1:J:98:ALA:O	1:J:100:GLU:HG3	2.15	0.46
1:L:182:TYR:HD2	1:L:257:TYR:CE2	2.34	0.46
1:N:7:ILE:HD12	1:N:116:SER:O	2.15	0.46
1:L:152:LEU:HD23	1:L:152:LEU:HA	1.79	0.46
1:N:159:GLU:OE1	1:N:159:GLU:N	2.39	0.46
1:A:157:LEU:HD23	1:A:161:TYR:HE2	1.81	0.45
1:B:9:TYR:HB2	1:B:83:SER:HB3	1.97	0.45
1:D:37:ILE:HA	1:D:96:GLU:OE1	2.17	0.45
1:D:146:LEU:HB2	1:D:268:ARG:O	2.16	0.45
1:F:138:ARG:HH21	1:F:242:GLU:CD	2.25	0.45
1:H:153:LEU:HD21	1:H:158:SER:HA	1.98	0.45
1:J:26:VAL:HG23	1:J:27:LEU:H	1.79	0.45
1:J:41:LYS:HG2	1:J:42:ASP:H	1.81	0.45
1:J:60:PHE:HB3	1:J:65:ILE:HD11	1.98	0.45
1:N:26:VAL:HG13	1:N:27:LEU:H	1.82	0.45
1:N:147:LEU:HD21	1:N:177:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:232:ARG:HH12	2:O:7:C:H1'	1.81	0.45
1:B:38:PRO:C	1:B:40:LEU:H	2.25	0.45
1:B:226:ASP:HA	1:B:227:SER:HA	1.72	0.45
1:F:73:LYS:HG3	1:F:74:THR:N	2.30	0.45
1:H:17:VAL:HG21	1:H:107:TYR:O	2.16	0.45
1:A:284:ILE:H	1:A:284:ILE:HG13	1.40	0.45
1:F:93:VAL:HG12	1:F:97:VAL:HG13	1.98	0.45
1:H:6:LYS:HE3	1:H:84:ILE:HG23	1.97	0.45
1:A:14:LEU:O	1:A:77:LYS:HG3	2.16	0.45
1:B:228:LYS:HA	1:B:229:GLY:HA2	1.66	0.45
2:C:7:C:C4	2:C:8:U:C4	3.05	0.45
1:D:55:ILE:O	1:D:55:ILE:HG13	2.15	0.45
1:F:30:LEU:O	1:F:30:LEU:HD23	2.17	0.45
1:L:14:LEU:HD12	1:L:109:LYS:HB3	1.98	0.45
1:L:55:ILE:HG22	1:L:85:ILE:HG23	1.98	0.45
1:N:157:LEU:N	1:N:157:LEU:HD12	2.31	0.45
1:N:255:LEU:O	1:N:259:LEU:HB3	2.16	0.45
1:H:174:VAL:O	1:H:177:ILE:HG13	2.17	0.45
1:A:15:GLN:HE22	1:A:109:LYS:H	1.63	0.45
1:D:13:PRO:HB3	1:D:110:PHE:CZ	2.52	0.45
1:D:46:SER:O	1:D:51:LYS:NZ	2.39	0.45
1:H:182:TYR:CE2	1:H:194:VAL:HG12	2.51	0.45
1:L:17:VAL:O	1:L:75:ILE:HD13	2.16	0.45
1:J:15:GLN:O	1:J:77:LYS:HG3	2.16	0.45
1:L:12:ILE:CD1	1:L:80:ARG:HA	2.47	0.45
1:L:267:GLY:O	1:L:270:ARG:NH1	2.42	0.45
1:A:55:ILE:HG22	1:A:85:ILE:HB	1.99	0.45
1:H:42:ASP:O	1:H:45:THR:HG22	2.16	0.45
1:J:223:ILE:HB	1:J:224:GLY:H	1.61	0.45
1:L:146:LEU:HB3	1:L:168:TYR:CE1	2.52	0.45
1:L:235:ARG:CZ	2:M:4:A:H5''	2.46	0.45
1:A:23:SER:HB2	1:A:58:LEU:HD12	1.99	0.45
1:A:172:PRO:HG3	1:A:237:VAL:HG11	1.99	0.45
1:J:23:SER:O	1:J:26:VAL:HG22	2.17	0.45
1:J:163:LYS:HA	1:J:163:LYS:HD3	1.67	0.45
1:L:222:ALA:O	1:L:223:ILE:HD13	2.17	0.45
1:L:84:ILE:HD12	1:L:278:ARG:HH22	1.82	0.44
1:L:143:SER:HB3	1:L:276:GLU:HB3	1.99	0.44
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.82	0.44
1:D:233:LYS:HE2	2:E:6:U:OP1	2.17	0.44
1:F:40:LEU:HD21	1:F:87:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:GLU:O	1:F:131:LYS:HG2	2.16	0.44
1:J:212:ILE:HD11	1:J:242:GLU:HG2	1.98	0.44
1:L:48:ASP:HA	2:M:11:U:N3	2.32	0.44
1:N:161:TYR:HD2	1:N:164:ILE:HD12	1.82	0.44
1:B:118:GLU:O	1:B:119:ILE:HD13	2.17	0.44
1:B:249:ARG:HH21	1:B:253:ARG:NH1	2.15	0.44
1:L:151:VAL:HG21	1:L:180:TYR:CZ	2.53	0.44
1:N:11:VAL:O	1:N:81:LEU:HB2	2.18	0.44
1:A:217:HIS:HA	1:A:218:PRO:HD3	1.87	0.44
1:B:11:VAL:O	1:B:81:LEU:HB2	2.18	0.44
1:N:197:ARG:HH21	1:N:253:ARG:NH2	2.06	0.44
1:F:43:LEU:HB2	1:F:53:ILE:CD1	2.47	0.44
1:A:113:MET:HG2	1:A:114:ILE:H	1.82	0.44
1:D:195:GLU:OE1	1:D:195:GLU:N	2.41	0.44
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.87	0.44
1:F:210:ARG:HH21	1:F:246:PRO:HG3	1.83	0.44
1:A:214:TYR:HB2	1:A:216:LEU:CD2	2.47	0.44
1:B:47:ARG:NH1	2:C:9:A:C8	2.86	0.44
1:B:242:GLU:OE2	1:B:282:ARG:NH1	2.50	0.44
1:F:40:LEU:HD21	1:F:87:PHE:HE1	1.82	0.44
1:F:255:LEU:O	1:F:259:LEU:HG	2.18	0.44
1:H:22:PRO:HG2	1:H:272:ILE:CG2	2.48	0.44
1:H:28:LYS:HD2	1:H:44:ILE:HD13	2.00	0.44
1:J:144:PRO:HG3	1:J:238:MET:HE1	1.98	0.44
1:J:155:PRO:O	1:J:158:SER:HB3	2.18	0.44
1:A:145:THR:HG22	1:A:147:LEU:HD13	2.00	0.44
1:B:84:ILE:O	1:B:85:ILE:HD12	2.18	0.44
1:B:99:ASP:HB3	1:B:103:PHE:CZ	2.53	0.44
1:B:162:LYS:HG3	1:B:163:LYS:N	2.33	0.44
2:C:7:C:N4	2:C:8:U:O4	2.51	0.44
1:D:40:LEU:CG	1:D:43:LEU:HD11	2.44	0.44
1:J:225:GLU:CD	1:J:230:ASN:N	2.75	0.44
1:J:238:MET:HE2	1:J:238:MET:HB2	1.69	0.44
1:A:97:VAL:HG23	1:A:98:ALA:H	1.83	0.43
1:D:194:VAL:N	1:D:195:GLU:OE1	2.50	0.43
1:H:51:LYS:HG3	1:H:53:ILE:HG22	1.99	0.43
1:J:21:THR:HG23	1:J:67:GLN:OE1	2.18	0.43
1:J:185:TYR:CD1	1:J:260:THR:HG21	2.53	0.43
1:N:155:PRO:HG2	1:N:196:VAL:HA	2.00	0.43
1:B:37:ILE:HG12	1:B:97:VAL:H	1.84	0.43
1:H:5:PHE:HD2	1:H:119:ILE:HG12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:THR:HG22	1:H:107:TYR:H	1.82	0.43
1:J:154:PRO:HB2	1:J:157:LEU:HD22	1.99	0.43
1:L:65:ILE:H	1:L:65:ILE:HG13	1.67	0.43
1:A:185:TYR:O	1:A:188:LEU:HB3	2.18	0.43
1:D:94:LEU:HD12	1:D:94:LEU:H	1.84	0.43
1:F:247:ASP:HB2	1:J:164:ILE:HD13	2.00	0.43
1:N:35:LYS:HG2	1:N:103:PHE:CD1	2.54	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.81	0.43
1:D:67:GLN:HG2	1:D:222:ALA:HB3	2.00	0.43
1:D:279:LEU:HD22	1:D:281:PHE:CZ	2.53	0.43
1:H:139:VAL:HG22	1:H:277:ILE:HD12	2.00	0.43
1:J:212:ILE:HD12	1:J:213:GLY:N	2.33	0.43
1:J:232:ARG:NH1	2:K:7:C:O2	2.52	0.43
1:L:21:THR:O	1:L:25:LYS:NZ	2.51	0.43
1:L:104:GLU:HB3	1:L:109:LYS:HD3	2.00	0.43
1:N:197:ARG:NH2	1:N:201:PHE:HB2	2.33	0.43
1:F:57:HIS:O	1:F:64:ARG:HD2	2.18	0.43
1:L:171:LEU:HD23	1:L:171:LEU:HA	1.79	0.43
1:N:197:ARG:NH2	1:N:253:ARG:HH12	2.17	0.43
1:A:154:PRO:HB2	1:A:157:LEU:HD13	2.00	0.43
1:D:151:VAL:HG21	1:D:180:TYR:CZ	2.54	0.43
2:G:4:A:H4'	2:G:5:A:OP1	2.18	0.43
1:H:201:PHE:CE1	1:H:250:LEU:HD13	2.54	0.43
1:J:195:GLU:H	1:J:195:GLU:HG3	1.62	0.43
1:N:266:ILE:HD12	1:N:266:ILE:HA	1.66	0.43
1:F:8:GLY:HA2	1:F:84:ILE:HD13	1.99	0.43
1:F:40:LEU:HA	1:F:43:LEU:HG	1.99	0.43
1:F:73:LYS:CG	1:F:74:THR:H	2.32	0.43
1:J:214:TYR:HB2	1:J:216:LEU:CD2	2.49	0.43
1:B:192:LYS:HB3	1:B:193:GLU:H	1.54	0.43
1:F:224:GLY:HA3	1:F:232:ARG:HH21	1.82	0.43
1:H:44:ILE:HG22	1:H:53:ILE:HD13	2.01	0.43
1:J:247:ASP:OD2	1:J:250:LEU:HB2	2.18	0.43
1:N:25:LYS:HA	1:N:28:LYS:HB3	2.00	0.43
1:N:60:PHE:CG	1:N:61:ASN:N	2.86	0.43
1:N:174:VAL:O	1:N:177:ILE:HG12	2.19	0.43
1:A:36:LEU:O	1:A:37:ILE:C	2.61	0.43
1:B:77:LYS:O	1:B:79:SER:OG	2.37	0.43
1:B:133:MET:C	1:B:251:LYS:HE2	2.44	0.43
1:F:40:LEU:HG	1:F:43:LEU:HD11	2.01	0.43
1:H:272:ILE:O	1:H:272:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:17:VAL:H	1:N:75:ILE:HG22	1.83	0.43
1:B:47:ARG:NH2	2:C:11:U:H5	2.16	0.43
1:B:230:ASN:HB3	1:B:231:LEU:H	1.56	0.43
1:D:38:PRO:HD2	1:D:96:GLU:CD	2.43	0.43
2:E:4:A:H1'	2:E:5:A:H2'	2.01	0.43
1:H:40:LEU:HD11	1:H:87:PHE:CD1	2.54	0.43
1:H:93:VAL:O	1:H:95:SER:N	2.51	0.43
1:J:25:LYS:O	1:J:28:LYS:HB3	2.19	0.43
1:L:154:PRO:HA	1:L:155:PRO:HD3	1.80	0.43
1:B:26:VAL:HG23	1:B:27:LEU:H	1.84	0.42
1:D:48:ASP:HA	2:E:11:U:C2	2.54	0.42
1:F:40:LEU:O	1:F:43:LEU:HG	2.19	0.42
1:D:146:LEU:HD12	1:D:168:TYR:CD2	2.54	0.42
1:J:61:ASN:OD1	1:J:61:ASN:C	2.62	0.42
1:L:41:LYS:HA	1:L:41:LYS:HD3	1.76	0.42
1:L:129:VAL:HG11	1:L:252:ARG:HG3	2.01	0.42
1:B:270:ARG:NH2	2:C:15:G:OP1	2.36	0.42
1:D:159:GLU:O	1:D:162:LYS:HG3	2.19	0.42
1:N:22:PRO:HG2	1:N:272:ILE:HG13	2.01	0.42
1:A:88:SER:O	1:A:89:THR:HG23	2.19	0.42
1:A:258:LEU:HB3	1:A:279:LEU:HD11	2.00	0.42
1:B:21:THR:O	1:B:25:LYS:HE3	2.19	0.42
1:B:53:ILE:HD12	1:B:87:PHE:HB3	2.01	0.42
1:D:154:PRO:HA	1:D:155:PRO:HD3	1.77	0.42
1:H:248:GLU:OE2	1:H:248:GLU:N	2.51	0.42
1:N:158:SER:O	1:N:162:LYS:HE3	2.19	0.42
1:F:9:TYR:OH	1:F:36:LEU:HD11	2.19	0.42
1:J:186:CYS:O	1:J:190:GLY:N	2.53	0.42
1:N:128:GLU:HG3	1:N:131:LYS:HE2	2.01	0.42
1:B:214:TYR:HB2	1:B:216:LEU:CD2	2.50	0.42
1:D:14:LEU:HD11	1:D:109:LYS:HB3	2.02	0.42
1:D:120:VAL:HG11	1:D:125:LEU:HD21	2.00	0.42
1:D:221:VAL:HG21	1:D:274:PHE:CE1	2.54	0.42
2:E:14:A:H2'	2:E:15:G:C8	2.54	0.42
1:J:27:LEU:HD12	1:J:30:LEU:HD12	2.01	0.42
1:N:250:LEU:HA	1:N:250:LEU:HD23	1.84	0.42
1:A:214:TYR:HB2	1:A:216:LEU:HD22	2.00	0.42
1:B:217:HIS:HA	1:B:218:PRO:HD3	1.93	0.42
1:B:232:ARG:HH22	1:B:234:ALA:N	2.17	0.42
1:H:154:PRO:HA	1:H:155:PRO:HD3	1.90	0.42
1:H:206:ASN:HA	1:H:209:SER:HG	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:C	1:A:119:ILE:HD12	2.45	0.42
1:A:207:ALA:HB1	1:B:153:LEU:HB2	2.02	0.42
1:B:232:ARG:NH1	1:B:233:LYS:O	2.51	0.42
1:D:14:LEU:O	1:D:77:LYS:HG3	2.20	0.42
1:D:56:SER:OG	1:D:64:ARG:NH2	2.52	0.42
1:D:185:TYR:O	1:D:188:LEU:HB3	2.20	0.42
1:D:233:LYS:HZ1	2:E:6:U:H5'	1.81	0.42
1:H:9:TYR:CE2	1:H:112:ILE:HD11	2.55	0.42
1:L:258:LEU:HD23	1:L:258:LEU:HA	1.80	0.42
1:N:232:ARG:NE	2:O:16:A:C2	2.86	0.42
1:A:222:ALA:C	1:A:223:ILE:HD13	2.45	0.42
1:B:87:PHE:N	1:B:87:PHE:CD1	2.88	0.42
1:B:282:ARG:HE	1:B:282:ARG:HB3	1.53	0.42
1:F:171:LEU:HD12	1:F:171:LEU:HA	1.84	0.42
1:J:126:LYS:HG2	1:J:256:ASN:OD1	2.20	0.42
1:N:19:LEU:H	1:N:19:LEU:HG	1.60	0.42
1:B:249:ARG:HH21	1:B:253:ARG:HH11	1.68	0.42
1:D:11:VAL:HG13	1:D:81:LEU:HB2	2.01	0.42
1:D:30:LEU:HB3	1:D:36:LEU:HD21	2.02	0.42
1:D:145:THR:HG22	1:D:147:LEU:HD13	2.01	0.42
1:F:258:LEU:HD23	1:F:258:LEU:HA	1.83	0.42
1:A:220:THR:HG23	2:R:5:A:H5''	2.01	0.41
1:H:31:ILE:CD1	1:H:37:ILE:HG23	2.50	0.41
1:H:58:LEU:HD12	1:H:83:SER:OG	2.20	0.41
2:I:9:A:O3'	2:I:10:C:H4'	2.20	0.41
1:J:95:SER:OG	1:J:96:GLU:N	2.52	0.41
1:A:244:ASP:OD1	1:A:251:LYS:NZ	2.53	0.41
1:B:151:VAL:HG21	1:B:180:TYR:CZ	2.55	0.41
1:D:9:TYR:CZ	1:D:85:ILE:HD11	2.55	0.41
1:D:57:HIS:O	1:D:64:ARG:NH2	2.52	0.41
1:D:233:LYS:CE	2:E:6:U:H5'	2.49	0.41
1:F:146:LEU:HB3	1:F:168:TYR:CE1	2.54	0.41
1:N:63:ARG:NH1	1:N:63:ARG:HG3	2.35	0.41
1:N:146:LEU:HB2	1:N:268:ARG:O	2.19	0.41
1:A:169:SER:C	1:A:171:LEU:H	2.27	0.41
1:D:38:PRO:C	1:D:40:LEU:N	2.77	0.41
1:J:192:LYS:HD2	1:J:192:LYS:HA	1.48	0.41
1:N:31:ILE:O	1:N:33:SER:N	2.49	0.41
1:B:120:VAL:HG23	1:B:124:LYS:NZ	2.36	0.41
1:H:105:THR:HG22	1:H:106:VAL:N	2.35	0.41
1:H:175:GLY:N	1:H:206:ASN:HB3	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:GLY:HA3	1:J:230:ASN:HA	1.81	0.41
1:L:38:PRO:CA	1:L:41:LYS:HE2	2.50	0.41
1:L:268:ARG:HA	1:L:269:SER:HA	1.87	0.41
2:E:15:G:H2'	2:E:16:A:H8	1.83	0.41
1:H:96:GLU:O	1:H:97:VAL:C	2.62	0.41
1:H:233:LYS:HG2	2:I:6:U:H5'	2.02	0.41
1:N:232:ARG:HH21	2:O:16:A:H2	1.64	0.41
1:A:152:LEU:HD22	1:A:203:ILE:HD13	2.01	0.41
1:F:47:ARG:HA	2:G:15:G:H4'	2.02	0.41
1:H:140:ARG:O	1:H:277:ILE:HA	2.21	0.41
1:J:220:THR:OG1	1:J:235:ARG:NH1	2.54	0.41
1:L:168:TYR:OH	1:L:268:ARG:HD2	2.21	0.41
1:L:25:LYS:O	1:L:28:LYS:HB3	2.21	0.41
1:L:180:TYR:CE1	1:L:267:GLY:HA2	2.56	0.41
1:A:29:TYR:CD2	1:A:29:TYR:C	2.99	0.41
1:B:1:MET:CB	1:J:193:GLU:HG3	2.50	0.41
1:B:249:ARG:HD3	1:B:250:LEU:N	2.36	0.41
1:B:279:LEU:HD23	1:B:279:LEU:HA	1.93	0.41
1:D:7:ILE:HG12	1:D:9:TYR:CE2	2.56	0.41
1:F:14:LEU:HD13	1:F:14:LEU:HA	1.92	0.41
1:F:16:ASP:N	1:F:77:LYS:HD3	2.36	0.41
1:N:10:ASN:HB3	1:N:80:ARG:NH1	2.36	0.41
2:O:7:C:H42	2:O:14:A:N6	2.18	0.41
1:B:121:GLU:H	1:B:121:GLU:HG2	1.72	0.41
1:B:232:ARG:NE	2:C:6:U:O2	2.54	0.41
1:D:21:THR:HA	1:D:22:PRO:HA	1.88	0.41
1:D:152:LEU:HD22	1:D:176:LEU:HG	2.03	0.41
1:D:225:GLU:HG3	1:D:232:ARG:NE	2.36	0.41
1:F:22:PRO:HD3	1:F:223:ILE:O	2.21	0.41
1:F:51:LYS:HE3	2:G:15:G:H5''	2.03	0.41
1:F:51:LYS:NZ	2:G:16:A:OP1	2.53	0.41
1:F:268:ARG:HA	1:F:269:SER:HA	1.81	0.41
1:H:4:ILE:HA	1:H:88:SER:HG	1.85	0.41
1:J:15:GLN:NE2	1:J:109:LYS:H	2.19	0.41
1:J:26:VAL:HG23	1:J:27:LEU:N	2.36	0.41
1:L:13:PRO:HB3	1:L:110:PHE:CE1	2.56	0.41
1:L:20:PRO:HG2	1:L:25:LYS:HB2	2.02	0.41
1:L:217:HIS:HA	1:L:218:PRO:HD3	1.88	0.41
1:L:222:ALA:C	1:L:223:ILE:HD13	2.46	0.41
1:N:138:ARG:HH21	1:N:242:GLU:CD	2.29	0.41
1:N:185:TYR:CD2	1:N:260:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:C	1:A:40:LEU:H	2.29	0.41
1:B:121:GLU:HG3	1:B:124:LYS:HB3	2.03	0.41
1:B:258:LEU:HB3	1:B:279:LEU:HD11	2.02	0.41
1:D:93:VAL:O	1:D:95:SER:N	2.54	0.41
1:F:140:ARG:HG3	1:F:240:TRP:HB3	2.03	0.41
1:N:195:GLU:CD	1:N:195:GLU:H	2.28	0.41
1:B:37:ILE:HA	1:B:38:PRO:HD2	1.89	0.40
1:F:34:GLY:N	1:F:41:LYS:NZ	2.69	0.40
1:F:191:LYS:O	1:F:192:LYS:HD3	2.20	0.40
1:L:139:VAL:HG13	1:L:241:ILE:HG23	2.02	0.40
1:D:157:LEU:HD23	1:D:161:TYR:HE1	1.86	0.40
2:G:4:A:H62	1:J:136:ASN:CG	2.27	0.40
1:H:127:GLU:HG2	1:H:128:GLU:N	2.35	0.40
1:J:87:PHE:N	1:J:87:PHE:CD2	2.90	0.40
1:L:76:THR:OG1	1:L:77:LYS:N	2.54	0.40
2:M:4:A:H4'	2:M:5:A:OP1	2.21	0.40
1:H:11:VAL:O	1:H:81:LEU:HB2	2.21	0.40
1:H:192:LYS:HD2	1:H:192:LYS:HA	1.56	0.40
1:H:271:GLY:C	1:H:272:ILE:HG13	2.46	0.40
1:L:67:GLN:N	1:L:67:GLN:HE21	2.19	0.40
1:A:14:LEU:HD12	1:A:109:LYS:HD2	2.04	0.40
1:A:268:ARG:HA	1:A:269:SER:HA	1.86	0.40
1:F:162:LYS:NZ	2:G:10:C:O2	2.54	0.40
1:J:125:LEU:HD21	1:J:260:THR:HG22	2.03	0.40
1:D:42:ASP:O	1:D:46:SER:N	2.54	0.40
1:H:128:GLU:OE2	1:H:259:LEU:HD13	2.22	0.40
1:H:136:ASN:O	1:H:281:PHE:HA	2.21	0.40
1:L:15:GLN:O	1:L:77:LYS:HA	2.21	0.40

All (3) 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)
2:E:2:C:OP1	1:N:63:ARG:NH1[1_655]	1.93	0.27
1:A:63:ARG:NH2	2:G:3:U:OP2[2_657]	2.09	0.11
2:C:2:C:OP1	1:J:63:ARG:NH2[2_657]	2.11	0.09

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	273/289 (94%)	250 (92%)	12 (4%)	11 (4%)	2	11
1	B	277/289 (96%)	255 (92%)	12 (4%)	10 (4%)	2	12
1	D	270/289 (93%)	246 (91%)	14 (5%)	10 (4%)	2	12
1	F	272/289 (94%)	250 (92%)	9 (3%)	13 (5%)	2	9
1	H	270/289 (93%)	250 (93%)	12 (4%)	8 (3%)	3	15
1	J	279/289 (96%)	248 (89%)	15 (5%)	16 (6%)	1	6
1	L	272/289 (94%)	247 (91%)	17 (6%)	8 (3%)	3	16
1	N	268/289 (93%)	239 (89%)	19 (7%)	10 (4%)	2	12
All	All	2181/2312 (94%)	1985 (91%)	110 (5%)	86 (4%)	2	11

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	68	THR
1	A	94	LEU
1	A	99	ASP
1	D	61	ASN
1	D	94	LEU
1	D	99	ASP
1	F	61	ASN
1	F	68	THR
1	F	74	THR
1	F	94	LEU
1	F	99	ASP
1	H	61	ASN
1	H	94	LEU
1	H	99	ASP
1	J	61	ASN
1	J	62	GLN

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Mol	Chain	Res	Type
1	J	68	THR
1	J	80	ARG
1	J	94	LEU
1	J	97	VAL
1	J	99	ASP
1	L	61	ASN
1	L	96	GLU
1	N	94	LEU
1	N	96	GLU
1	N	99	ASP
1	B	68	THR
1	B	226	ASP
1	D	233	LYS
1	F	39	SER
1	F	226	ASP
1	H	68	THR
1	H	97	VAL
1	J	75	ILE
1	J	223	ILE
1	L	94	LEU
1	L	99	ASP
1	N	193	GLU
1	A	193	GLU
1	B	61	ASN
1	B	89	THR
1	B	99	ASP
1	B	231	LEU
1	D	68	THR
1	D	78	GLY
1	H	96	GLU
1	J	192	LYS
1	J	227	SER
1	A	96	GLU
1	A	97	VAL
1	A	226	ASP
1	B	77	LYS
1	B	97	VAL
1	D	96	GLU
1	D	100	GLU
1	F	65	ILE
1	F	96	GLU
1	F	97	VAL

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Mol	Chain	Res	Type
1	J	74	THR
1	J	96	GLU
1	J	116	SER
1	J	190	GLY
1	L	100	GLU
1	L	193	GLU
1	N	32	GLN
1	N	79	SER
1	N	89	THR
1	N	97	VAL
1	A	37	ILE
1	A	65	ILE
1	A	89	THR
1	B	37	ILE
1	F	41	LYS
1	F	100	GLU
1	H	100	GLU
1	D	97	VAL
1	F	89	THR
1	H	37	ILE
1	J	231	LEU
1	L	39	SER
1	N	95	SER
1	B	65	ILE
1	D	37	ILE
1	N	37	ILE
1	L	97	VAL

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	246/256 (96%)	184 (75%)	62 (25%)	0	2
1	B	249/256 (97%)	193 (78%)	56 (22%)	1	3
1	D	245/256 (96%)	184 (75%)	61 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	247/256 (96%)	193 (78%)	54 (22%)	1	4
1	H	245/256 (96%)	190 (78%)	55 (22%)	1	3
1	J	251/256 (98%)	179 (71%)	72 (29%)	0	1
1	L	247/256 (96%)	186 (75%)	61 (25%)	1	2
1	N	243/256 (95%)	178 (73%)	65 (27%)	0	1
All	All	1973/2048 (96%)	1487 (75%)	486 (25%)	1	2

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	ASN
1	A	19	LEU
1	A	27	LEU
1	A	30	LEU
1	A	31	ILE
1	A	39	SER
1	A	44	ILE
1	A	63	ARG
1	A	67	GLN
1	A	68	THR
1	A	74	THR
1	A	75	ILE
1	A	76	THR
1	A	79	SER
1	A	80	ARG
1	A	81	LEU
1	A	83	SER
1	A	84	ILE
1	A	85	ILE
1	A	89	THR
1	A	93	VAL
1	A	94	LEU
1	A	96	GLU
1	A	114	ILE
1	A	120	VAL
1	A	124	LYS
1	A	130	GLU
1	A	133	MET
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	139	VAL
1	A	143	SER
1	A	146	LEU
1	A	147	LEU
1	A	149	SER
1	A	156	SER
1	A	157	LEU
1	A	162	LYS
1	A	163	LYS
1	A	165	HIS
1	A	171	LEU
1	A	174	VAL
1	A	184	VAL
1	A	186	CYS
1	A	189	ILE
1	A	192	LYS
1	A	197	ARG
1	A	203	ILE
1	A	204	LEU
1	A	205	SER
1	A	209	SER
1	A	210	ARG
1	A	219	VAL
1	A	223	ILE
1	A	231	LEU
1	A	250	LEU
1	A	262	SER
1	A	269	SER
1	A	270	ARG
1	A	272	ILE
1	A	279	LEU
1	A	284	ILE
1	B	4	ILE
1	B	6	LYS
1	B	7	ILE
1	B	19	LEU
1	B	24	SER
1	B	32	GLN
1	B	36	LEU
1	B	41	LYS
1	B	42	ASP
1	B	44	ILE

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Mol	Chain	Res	Type
1	B	46	SER
1	B	58	LEU
1	B	64	ARG
1	B	68	THR
1	B	73	LYS
1	B	75	ILE
1	B	77	LYS
1	B	79	SER
1	B	83	SER
1	B	84	ILE
1	B	85	ILE
1	B	87	PHE
1	B	90	GLN
1	B	94	LEU
1	B	96	GLU
1	B	100	GLU
1	B	117	ILE
1	B	124	LYS
1	B	125	LEU
1	B	128	GLU
1	B	143	SER
1	B	147	LEU
1	B	149	SER
1	B	156	SER
1	B	157	LEU
1	B	162	LYS
1	B	171	LEU
1	B	173	SER
1	B	174	VAL
1	B	184	VAL
1	B	186	CYS
1	B	197	ARG
1	B	200	LYS
1	B	203	ILE
1	B	219	VAL
1	B	221	VAL
1	B	223	ILE
1	B	231	LEU
1	B	232	ARG
1	B	248	GLU
1	B	249	ARG
1	B	259	LEU

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Mol	Chain	Res	Type
1	B	262	SER
1	B	266	ILE
1	B	269	SER
1	B	270	ARG
1	D	3	LEU
1	D	4	ILE
1	D	7	ILE
1	D	12	ILE
1	D	14	LEU
1	D	26	VAL
1	D	36	LEU
1	D	40	LEU
1	D	42	ASP
1	D	46	SER
1	D	48	ASP
1	D	66	PHE
1	D	76	THR
1	D	79	SER
1	D	82	SER
1	D	85	ILE
1	D	87	PHE
1	D	89	THR
1	D	96	GLU
1	D	97	VAL
1	D	102	ILE
1	D	106	VAL
1	D	113	MET
1	D	119	ILE
1	D	120	VAL
1	D	121	GLU
1	D	125	LEU
1	D	130	GLU
1	D	146	LEU
1	D	147	LEU
1	D	149	SER
1	D	152	LEU
1	D	156	SER
1	D	157	LEU
1	D	159	GLU
1	D	162	LYS
1	D	171	LEU
1	D	174	VAL

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Mol	Chain	Res	Type
1	D	176	LEU
1	D	186	CYS
1	D	194	VAL
1	D	197	ARG
1	D	203	ILE
1	D	204	LEU
1	D	209	SER
1	D	210	ARG
1	D	219	VAL
1	D	223	ILE
1	D	225	GLU
1	D	231	LEU
1	D	233	LYS
1	D	250	LEU
1	D	255	LEU
1	D	262	SER
1	D	269	SER
1	D	270	ARG
1	D	272	ILE
1	D	277	ILE
1	D	279	LEU
1	D	280	GLU
1	D	284	ILE
1	F	4	ILE
1	F	17	VAL
1	F	18	ILE
1	F	19	LEU
1	F	23	SER
1	F	27	LEU
1	F	33	SER
1	F	36	LEU
1	F	39	SER
1	F	40	LEU
1	F	41	LYS
1	F	42	ASP
1	F	44	ILE
1	F	46	SER
1	F	60	PHE
1	F	64	ARG
1	F	66	PHE
1	F	75	ILE
1	F	83	SER

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Mol	Chain	Res	Type
1	F	87	PHE
1	F	93	VAL
1	F	95	SER
1	F	97	VAL
1	F	102	ILE
1	F	106	VAL
1	F	114	ILE
1	F	119	ILE
1	F	124	LYS
1	F	125	LEU
1	F	143	SER
1	F	149	SER
1	F	152	LEU
1	F	156	SER
1	F	157	LEU
1	F	158	SER
1	F	160	ARG
1	F	171	LEU
1	F	176	LEU
1	F	188	LEU
1	F	189	ILE
1	F	203	ILE
1	F	209	SER
1	F	210	ARG
1	F	212	ILE
1	F	219	VAL
1	F	226	ASP
1	F	227	SER
1	F	237	VAL
1	F	256	ASN
1	F	262	SER
1	F	269	SER
1	F	270	ARG
1	F	277	ILE
1	F	279	LEU
1	H	3	LEU
1	H	4	ILE
1	H	11	VAL
1	H	14	LEU
1	H	19	LEU
1	H	21	THR
1	H	39	SER

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Mol	Chain	Res	Type
1	H	42	ASP
1	H	44	ILE
1	H	45	THR
1	H	58	LEU
1	H	74	THR
1	H	75	ILE
1	H	77	LYS
1	H	84	ILE
1	H	85	ILE
1	H	95	SER
1	H	97	VAL
1	H	106	VAL
1	H	111	HIS
1	H	114	ILE
1	H	115	GLU
1	H	117	ILE
1	H	130	GLU
1	H	133	MET
1	H	139	VAL
1	H	143	SER
1	H	146	LEU
1	H	147	LEU
1	H	149	SER
1	H	156	SER
1	H	157	LEU
1	H	158	SER
1	H	159	GLU
1	H	164	ILE
1	H	171	LEU
1	H	173	SER
1	H	174	VAL
1	H	176	LEU
1	H	180	TYR
1	H	192	LYS
1	H	194	VAL
1	H	195	GLU
1	H	203	ILE
1	H	204	LEU
1	H	205	SER
1	H	209	SER
1	H	219	VAL
1	H	223	ILE

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Mol	Chain	Res	Type
1	H	250	LEU
1	H	259	LEU
1	H	262	SER
1	H	269	SER
1	H	270	ARG
1	H	277	ILE
1	J	3	LEU
1	J	4	ILE
1	J	7	ILE
1	J	9	TYR
1	J	10	ASN
1	J	11	VAL
1	J	12	ILE
1	J	14	LEU
1	J	15	GLN
1	J	19	LEU
1	J	21	THR
1	J	24	SER
1	J	25	LYS
1	J	27	LEU
1	J	36	LEU
1	J	39	SER
1	J	40	LEU
1	J	42	ASP
1	J	44	ILE
1	J	46	SER
1	J	47	ARG
1	J	51	LYS
1	J	53	ILE
1	J	55	ILE
1	J	62	GLN
1	J	63	ARG
1	J	66	PHE
1	J	75	ILE
1	J	76	THR
1	J	82	SER
1	J	83	SER
1	J	85	ILE
1	J	87	PHE
1	J	93	VAL
1	J	100	GLU
1	J	102	ILE

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Mol	Chain	Res	Type
1	J	105	THR
1	J	106	VAL
1	J	114	ILE
1	J	117	ILE
1	J	131	LYS
1	J	137	ILE
1	J	147	LEU
1	J	156	SER
1	J	157	LEU
1	J	158	SER
1	J	171	LEU
1	J	173	SER
1	J	176	LEU
1	J	192	LYS
1	J	193	GLU
1	J	195	GLU
1	J	203	ILE
1	J	204	LEU
1	J	210	ARG
1	J	219	VAL
1	J	221	VAL
1	J	223	ILE
1	J	227	SER
1	J	228	LYS
1	J	231	LEU
1	J	235	ARG
1	J	238	MET
1	J	250	LEU
1	J	259	LEU
1	J	262	SER
1	J	266	ILE
1	J	268	ARG
1	J	269	SER
1	J	270	ARG
1	J	282	ARG
1	J	284	ILE
1	L	4	ILE
1	L	10	ASN
1	L	11	VAL
1	L	17	VAL
1	L	18	ILE
1	L	24	SER

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Mol	Chain	Res	Type
1	L	30	LEU
1	L	36	LEU
1	L	37	ILE
1	L	42	ASP
1	L	43	LEU
1	L	45	THR
1	L	46	SER
1	L	51	LYS
1	L	58	LEU
1	L	63	ARG
1	L	65	ILE
1	L	66	PHE
1	L	67	GLN
1	L	68	THR
1	L	75	ILE
1	L	83	SER
1	L	93	VAL
1	L	95	SER
1	L	97	VAL
1	L	100	GLU
1	L	104	GLU
1	L	109	LYS
1	L	114	ILE
1	L	115	GLU
1	L	119	ILE
1	L	120	VAL
1	L	139	VAL
1	L	146	LEU
1	L	149	SER
1	L	150	LYS
1	L	156	SER
1	L	158	SER
1	L	165	HIS
1	L	173	SER
1	L	174	VAL
1	L	189	ILE
1	L	194	VAL
1	L	203	ILE
1	L	204	LEU
1	L	205	SER
1	L	209	SER
1	L	219	VAL

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Mol	Chain	Res	Type
1	L	221	VAL
1	L	231	LEU
1	L	232	ARG
1	L	233	LYS
1	L	235	ARG
1	L	248	GLU
1	L	249	ARG
1	L	250	LEU
1	L	255	LEU
1	L	269	SER
1	L	270	ARG
1	L	277	ILE
1	L	279	LEU
1	N	3	LEU
1	N	4	ILE
1	N	7	ILE
1	N	11	VAL
1	N	17	VAL
1	N	18	ILE
1	N	19	LEU
1	N	25	LYS
1	N	26	VAL
1	N	27	LEU
1	N	32	GLN
1	N	37	ILE
1	N	39	SER
1	N	40	LEU
1	N	43	LEU
1	N	44	ILE
1	N	51	LYS
1	N	55	ILE
1	N	58	LEU
1	N	62	GLN
1	N	66	PHE
1	N	74	THR
1	N	83	SER
1	N	84	ILE
1	N	93	VAL
1	N	94	LEU
1	N	96	GLU
1	N	102	ILE
1	N	112	ILE

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Mol	Chain	Res	Type
1	N	114	ILE
1	N	125	LEU
1	N	130	GLU
1	N	137	ILE
1	N	139	VAL
1	N	143	SER
1	N	145	THR
1	N	149	SER
1	N	150	LYS
1	N	156	SER
1	N	157	LEU
1	N	159	GLU
1	N	171	LEU
1	N	173	SER
1	N	186	CYS
1	N	191	LYS
1	N	193	GLU
1	N	204	LEU
1	N	205	SER
1	N	209	SER
1	N	210	ARG
1	N	212	ILE
1	N	219	VAL
1	N	221	VAL
1	N	225	GLU
1	N	231	LEU
1	N	233	LYS
1	N	237	VAL
1	N	248	GLU
1	N	249	ARG
1	N	259	LEU
1	N	262	SER
1	N	266	ILE
1	N	269	SER
1	N	270	ARG
1	N	280	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	132	HIS

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Mol	Chain	Res	Type
1	A	206	ASN
1	B	32	GLN
1	B	111	HIS
1	B	134	ASN
1	B	165	HIS
1	F	206	ASN
1	H	15	GLN
1	H	92	ASN
1	H	187	ASN
1	J	10	ASN
1	J	206	ASN
1	J	217	HIS
1	L	67	GLN
1	L	183	ASN
1	N	15	GLN
1	N	32	GLN
1	N	187	ASN
1	N	206	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	15/16 (93%)	5 (33%)	1 (6%)
2	E	15/16 (93%)	7 (46%)	1 (6%)
2	G	15/16 (93%)	7 (46%)	1 (6%)
2	I	15/16 (93%)	8 (53%)	1 (6%)
2	K	15/16 (93%)	6 (40%)	0
2	M	15/16 (93%)	6 (40%)	0
2	O	15/16 (93%)	8 (53%)	2 (13%)
2	R	15/16 (93%)	7 (46%)	1 (6%)
All	All	120/128 (93%)	54 (45%)	7 (5%)

All (54) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	C
2	R	3	U
2	R	5	A
2	R	6	U
2	R	9	A
2	R	10	C

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Mol	Chain	Res	Type
2	R	16	A
2	C	5	A
2	C	6	U
2	C	9	A
2	C	10	C
2	C	16	A
2	E	2	C
2	E	3	U
2	E	4	A
2	E	5	A
2	E	9	A
2	E	10	C
2	E	14	A
2	G	2	C
2	G	3	U
2	G	5	A
2	G	6	U
2	G	9	A
2	G	10	C
2	G	16	A
2	I	2	C
2	I	3	U
2	I	4	A
2	I	5	A
2	I	6	U
2	I	9	A
2	I	10	C
2	I	16	A
2	K	5	A
2	K	6	U
2	K	9	A
2	K	10	C
2	K	14	A
2	K	15	G
2	M	4	A
2	M	5	A
2	M	6	U
2	M	9	A
2	M	10	C
2	M	14	A
2	O	2	C
2	O	3	U

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Mol	Chain	Res	Type
2	O	5	A
2	O	6	U
2	O	9	A
2	O	10	C
2	O	14	A
2	O	16	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	2	C
2	C	9	A
2	E	2	C
2	G	2	C
2	I	2	C
2	O	2	C
2	O	9	A

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 [i](#)

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	279/289 (96%)	-0.03	5 (1%) 67 45	20, 59, 107, 120	0
1	B	281/289 (97%)	-0.10	1 (0%) 88 75	19, 60, 108, 120	0
1	D	276/289 (95%)	-0.18	1 (0%) 88 75	24, 62, 111, 122	0
1	F	278/289 (96%)	-0.18	1 (0%) 88 75	22, 63, 109, 126	0
1	H	276/289 (95%)	-0.12	1 (0%) 88 75	22, 65, 109, 127	0
1	J	283/289 (97%)	-0.23	0 100 100	23, 63, 111, 124	0
1	L	278/289 (96%)	-0.29	1 (0%) 88 75	25, 66, 112, 121	0
1	N	274/289 (94%)	-0.14	0 100 100	28, 66, 111, 124	0
2	C	16/16 (100%)	-0.27	0 100 100	36, 55, 108, 134	0
2	E	16/16 (100%)	-0.26	0 100 100	41, 60, 111, 138	0
2	G	16/16 (100%)	-0.26	0 100 100	36, 60, 109, 139	0
2	I	16/16 (100%)	-0.45	0 100 100	41, 63, 111, 136	0
2	K	16/16 (100%)	-0.46	0 100 100	35, 61, 107, 140	0
2	M	16/16 (100%)	-0.60	0 100 100	41, 65, 112, 137	0
2	O	16/16 (100%)	-0.24	0 100 100	43, 67, 113, 138	0
2	R	16/16 (100%)	-0.37	0 100 100	36, 54, 104, 138	0
All	All	2353/2440 (96%)	-0.17	10 (0%) 88 75	19, 63, 111, 140	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	231	LEU	3.2
1	D	231	LEU	2.4
1	F	69	ASN	2.2
1	A	66	PHE	2.2
1	A	230	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	ASN	2.1
1	A	67	GLN	2.1
1	H	89	THR	2.1
1	B	76	THR	2.0
1	A	223	ILE	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.