



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 06:46 AM UTC

PDB ID : 6FL0 / pdb_00006fl0
Title : Crystal structure of the membrane attack complex assembly inhibitor BGA71 from Lyme disease agent *Borrelia burgdorferi*
Authors : Brangulis, K.; Akopjana, I.; Petrovskis, I.; Kazaks, A.; Tars, K.
Deposited on : 2018-01-25
Resolution : 2.90 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

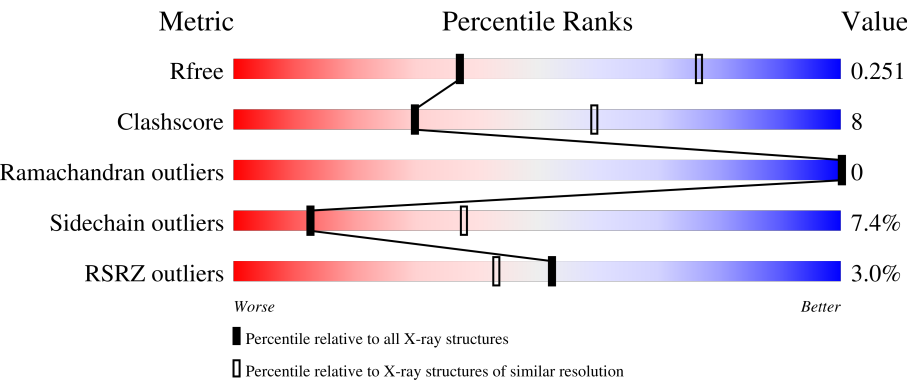
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	194	% 70% 23% • 6%
1	B	194	21% 74% 12% • 12%
1	C	194	3% 73% 19% • 7%
1	D	194	% 75% 16% • 6%
1	E	194	68% 23% • • 6%

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Mol	Chain	Length	Quality of chain
1	F	194	 % 61% 24% • • 11%
1	G	194	 % 72% 15% • 12%
1	H	194	 % 65% 22% •• 11%
1	I	194	 % 71% 19% • 7%
1	J	194	 74% 18% • 7%
1	K	194	 13% 67% 13% • 19%
1	L	194	 70% 21% • 7%
1	M	194	 2% 69% 18% • 12%
1	N	194	 % 56% 28% 5% 11%
1	O	194	 69% 22% • • 6%
1	P	194	 2% 65% 23% • 8%
1	Q	194	 % 64% 23% • 10%
1	R	194	 2% 59% 24% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26099 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 membrane attack complex assembly inhibitor BGA71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1517	956	253	304	4			
1	B	170	Total	C	N	O	S	0	0	0
			1332	837	224	268	3			
1	C	181	Total	C	N	O	S	0	0	0
			1503	947	251	301	4			
1	D	183	Total	C	N	O	S	0	0	0
			1517	956	253	304	4			
1	E	183	Total	C	N	O	S	0	0	0
			1514	953	253	304	4			
1	F	173	Total	C	N	O	S	0	0	0
			1434	908	237	285	4			
1	G	170	Total	C	N	O	S	0	0	0
			1411	895	232	280	4			
1	H	173	Total	C	N	O	S	0	0	0
			1433	906	236	287	4			
1	I	181	Total	C	N	O	S	0	0	0
			1502	947	250	301	4			
1	J	181	Total	C	N	O	S	0	0	0
			1503	947	251	301	4			
1	K	158	Total	C	N	O	S	0	0	0
			1268	795	215	254	4			
1	L	181	Total	C	N	O	S	0	0	0
			1503	947	251	301	4			
1	M	171	Total	C	N	O	S	0	0	0
			1418	897	233	284	4			
1	N	172	Total	C	N	O	S	0	0	0
			1425	901	234	286	4			
1	O	183	Total	C	N	O	S	0	0	0
			1514	953	253	304	4			
1	P	178	Total	C	N	O	S	0	0	0
			1475	931	244	296	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	175	Total	C	N	O	S	0	0	0
			1450	918	239	289	4			
1	R	166	Total	C	N	O	S	0	0	0
			1380	874	228	274	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP Q6ASF4
A	3	ALA	-	expression tag	UNP Q6ASF4
A	4	MET	-	expression tag	UNP Q6ASF4
A	5	GLY	-	expression tag	UNP Q6ASF4
B	2	GLY	-	expression tag	UNP Q6ASF4
B	3	ALA	-	expression tag	UNP Q6ASF4
B	4	MET	-	expression tag	UNP Q6ASF4
B	5	GLY	-	expression tag	UNP Q6ASF4
C	2	GLY	-	expression tag	UNP Q6ASF4
C	3	ALA	-	expression tag	UNP Q6ASF4
C	4	MET	-	expression tag	UNP Q6ASF4
C	5	GLY	-	expression tag	UNP Q6ASF4
D	2	GLY	-	expression tag	UNP Q6ASF4
D	3	ALA	-	expression tag	UNP Q6ASF4
D	4	MET	-	expression tag	UNP Q6ASF4
D	5	GLY	-	expression tag	UNP Q6ASF4
E	2	GLY	-	expression tag	UNP Q6ASF4
E	3	ALA	-	expression tag	UNP Q6ASF4
E	4	MET	-	expression tag	UNP Q6ASF4
E	5	GLY	-	expression tag	UNP Q6ASF4
F	2	GLY	-	expression tag	UNP Q6ASF4
F	3	ALA	-	expression tag	UNP Q6ASF4
F	4	MET	-	expression tag	UNP Q6ASF4
F	5	GLY	-	expression tag	UNP Q6ASF4
G	2	GLY	-	expression tag	UNP Q6ASF4
G	3	ALA	-	expression tag	UNP Q6ASF4
G	4	MET	-	expression tag	UNP Q6ASF4
G	5	GLY	-	expression tag	UNP Q6ASF4
H	2	GLY	-	expression tag	UNP Q6ASF4
H	3	ALA	-	expression tag	UNP Q6ASF4
H	4	MET	-	expression tag	UNP Q6ASF4
H	5	GLY	-	expression tag	UNP Q6ASF4
I	2	GLY	-	expression tag	UNP Q6ASF4
I	3	ALA	-	expression tag	UNP Q6ASF4

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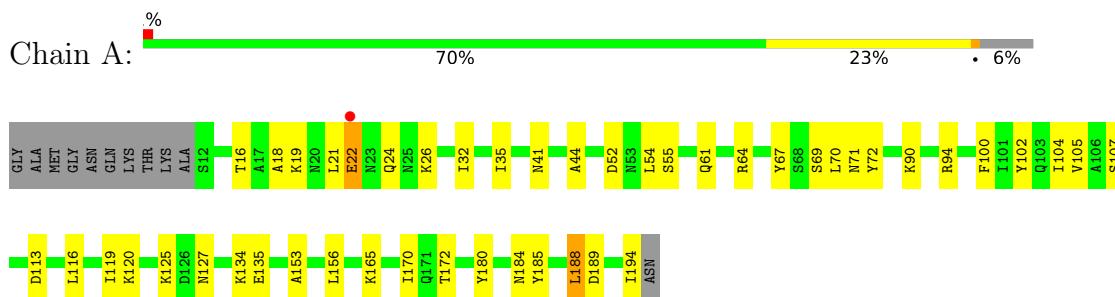
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Chain	Residue	Modelled	Actual	Comment	Reference
I	4	MET	-	expression tag	UNP Q6ASF4
I	5	GLY	-	expression tag	UNP Q6ASF4
J	2	GLY	-	expression tag	UNP Q6ASF4
J	3	ALA	-	expression tag	UNP Q6ASF4
J	4	MET	-	expression tag	UNP Q6ASF4
J	5	GLY	-	expression tag	UNP Q6ASF4
K	2	GLY	-	expression tag	UNP Q6ASF4
K	3	ALA	-	expression tag	UNP Q6ASF4
K	4	MET	-	expression tag	UNP Q6ASF4
K	5	GLY	-	expression tag	UNP Q6ASF4
L	2	GLY	-	expression tag	UNP Q6ASF4
L	3	ALA	-	expression tag	UNP Q6ASF4
L	4	MET	-	expression tag	UNP Q6ASF4
L	5	GLY	-	expression tag	UNP Q6ASF4
M	2	GLY	-	expression tag	UNP Q6ASF4
M	3	ALA	-	expression tag	UNP Q6ASF4
M	4	MET	-	expression tag	UNP Q6ASF4
M	5	GLY	-	expression tag	UNP Q6ASF4
N	2	GLY	-	expression tag	UNP Q6ASF4
N	3	ALA	-	expression tag	UNP Q6ASF4
N	4	MET	-	expression tag	UNP Q6ASF4
N	5	GLY	-	expression tag	UNP Q6ASF4
O	2	GLY	-	expression tag	UNP Q6ASF4
O	3	ALA	-	expression tag	UNP Q6ASF4
O	4	MET	-	expression tag	UNP Q6ASF4
O	5	GLY	-	expression tag	UNP Q6ASF4
P	2	GLY	-	expression tag	UNP Q6ASF4
P	3	ALA	-	expression tag	UNP Q6ASF4
P	4	MET	-	expression tag	UNP Q6ASF4
P	5	GLY	-	expression tag	UNP Q6ASF4
Q	2	GLY	-	expression tag	UNP Q6ASF4
Q	3	ALA	-	expression tag	UNP Q6ASF4
Q	4	MET	-	expression tag	UNP Q6ASF4
Q	5	GLY	-	expression tag	UNP Q6ASF4
R	2	GLY	-	expression tag	UNP Q6ASF4
R	3	ALA	-	expression tag	UNP Q6ASF4
R	4	MET	-	expression tag	UNP Q6ASF4
R	5	GLY	-	expression tag	UNP Q6ASF4

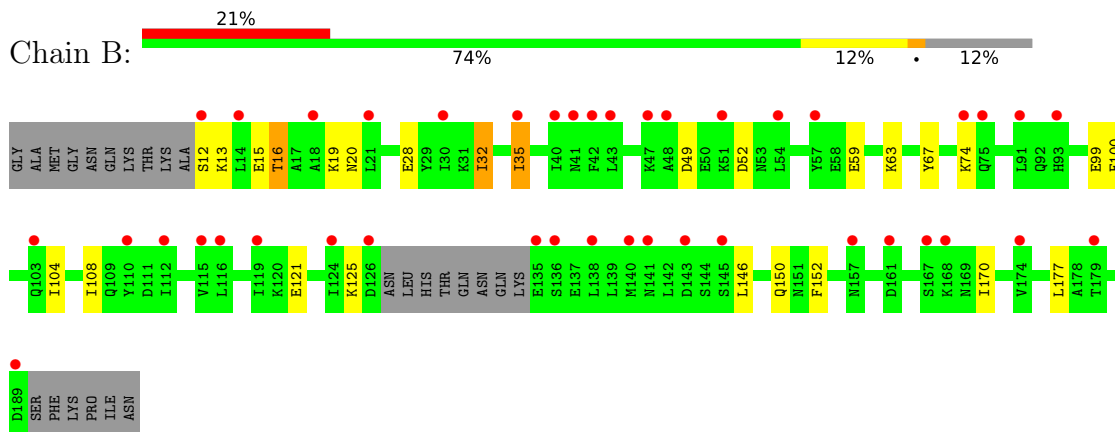
3 Residue-property plots

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.

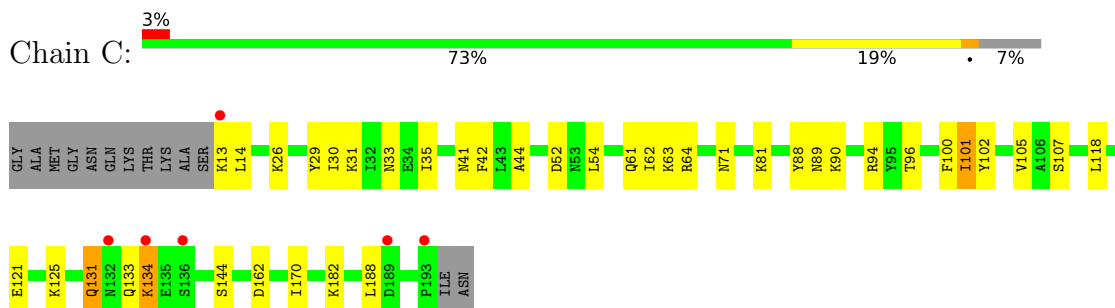
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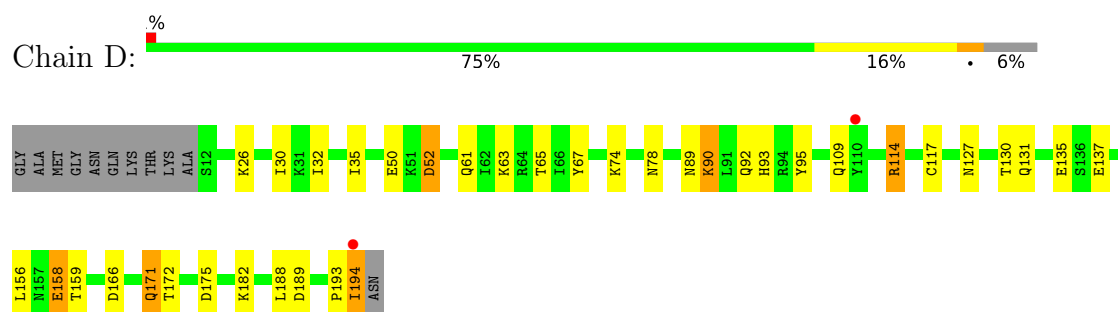
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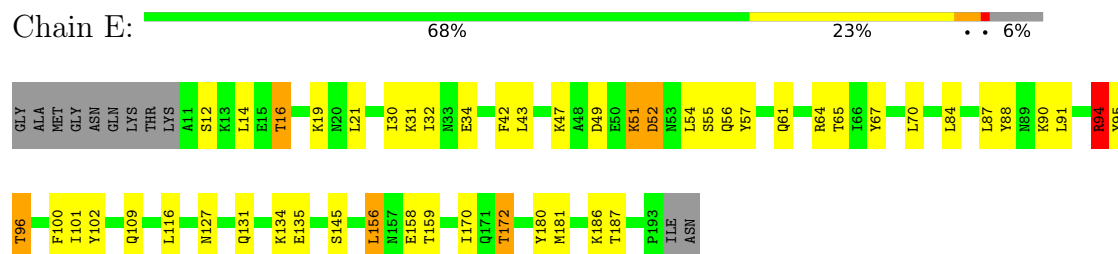
- Molecule 1: membrane attack complex assembly inhibitor BGA71



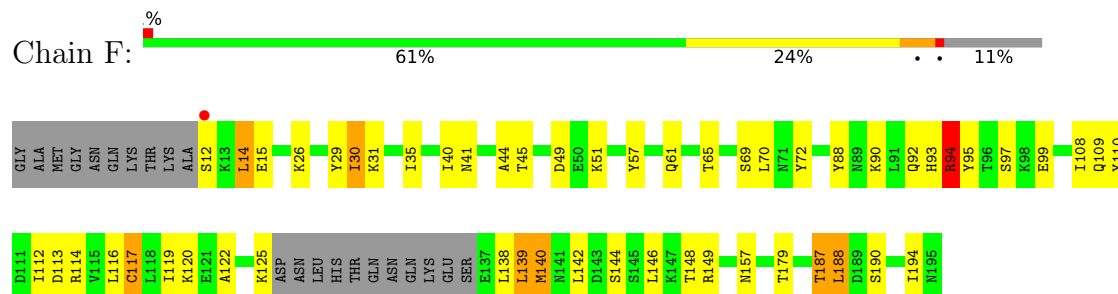
- Molecule 1: membrane attack complex assembly inhibitor BGA71



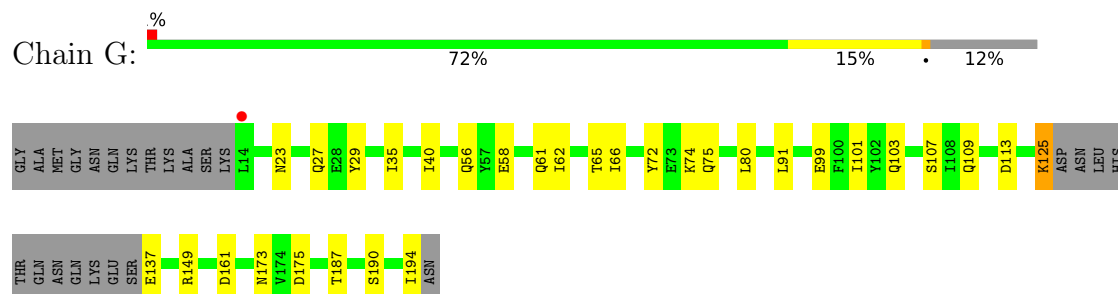
- Molecule 1: membrane attack complex assembly inhibitor BGA71



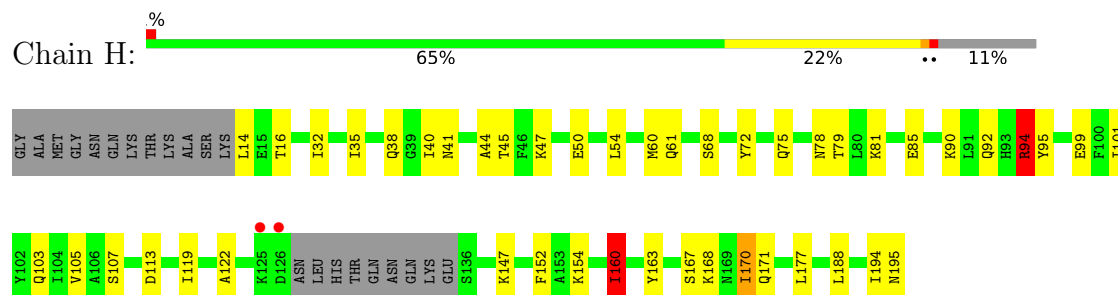
- Molecule 1: membrane attack complex assembly inhibitor BGA71



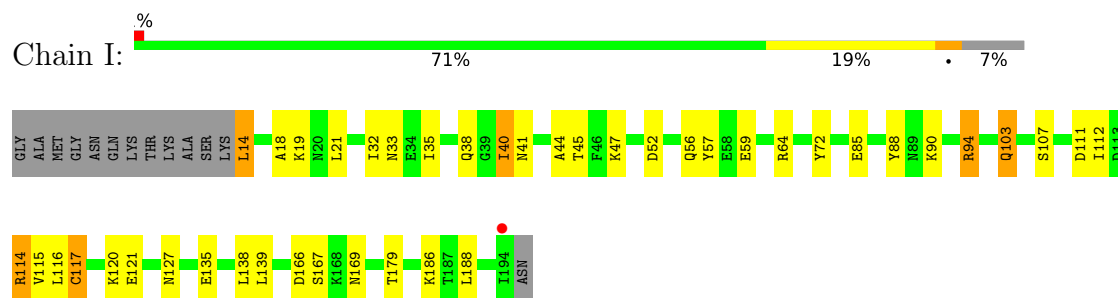
- Molecule 1: membrane attack complex assembly inhibitor BGA71



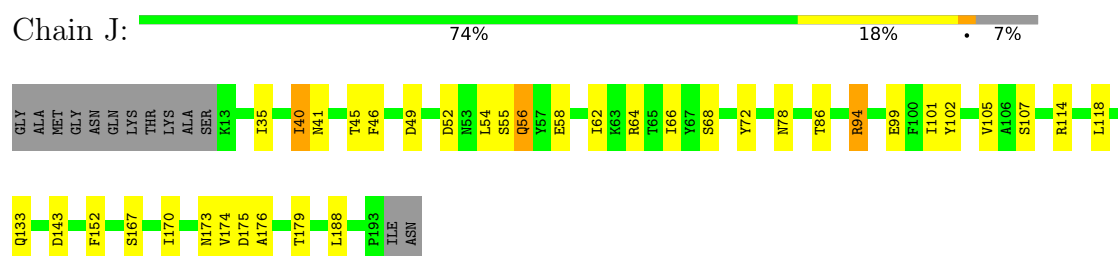
- Molecule 1: membrane attack complex assembly inhibitor BGA71



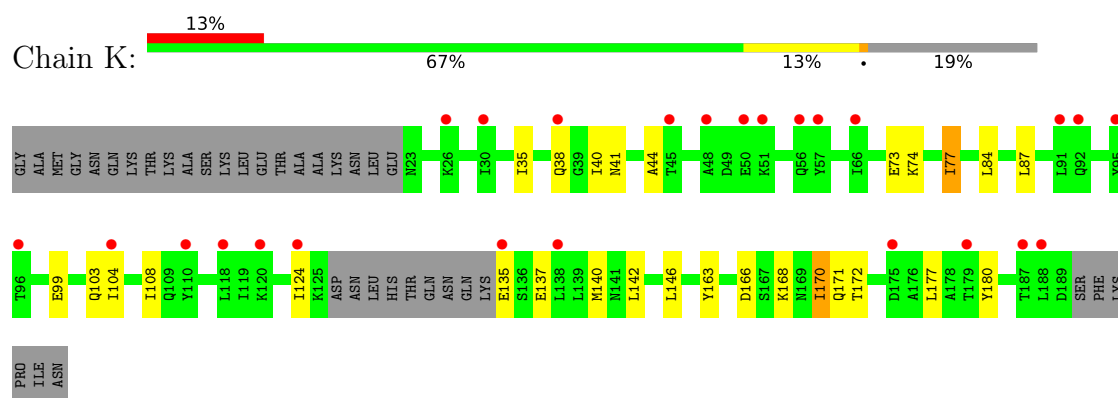
- Molecule 1: membrane attack complex assembly inhibitor BGA71



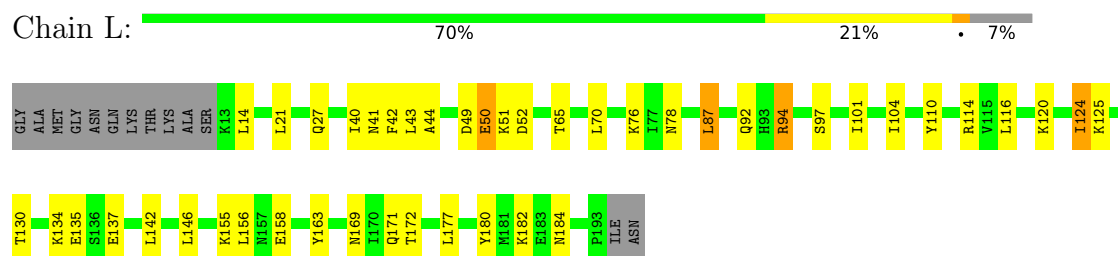
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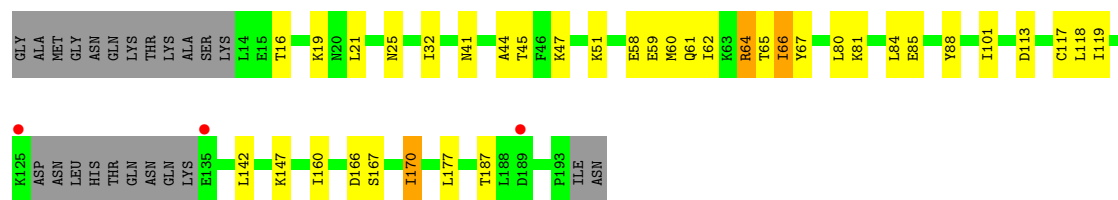


- Molecule 1: membrane attack complex assembly inhibitor BGA71

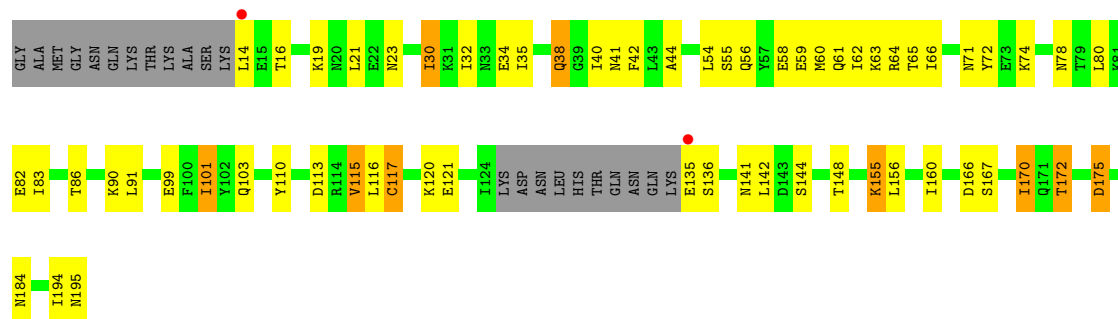


- Molecule 1: membrane attack complex assembly inhibitor BGA71

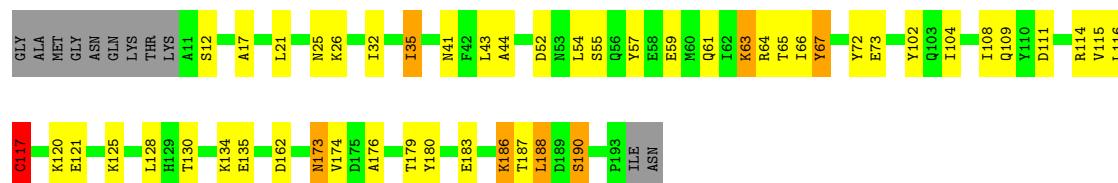




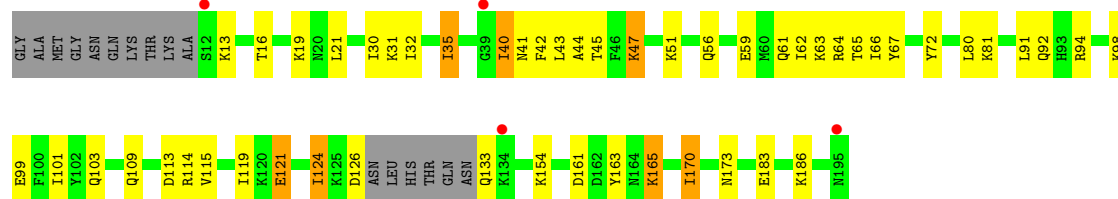
- Molecule 1: membrane attack complex assembly inhibitor BGA71



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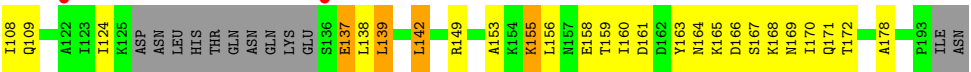


- Molecule 1: membrane attack complex assembly inhibitor BGA71





● Molecule 1: membrane attack complex assembly inhibitor BGA71



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	239.18Å 239.18Å 56.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.87 – 2.90 59.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (59.87-2.90) 99.9 (59.87-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.71 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.192 , 0.248 0.201 , 0.251	Depositor DCC
R_{free} test set	4045 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.005 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26099	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.71	0/1535	1.13	0/2062
1	B	0.58	0/1343	1.06	0/1808
1	C	0.61	0/1521	1.13	0/2043
1	D	0.68	0/1535	1.08	0/2062
1	E	0.77	1/1532 (0.1%)	1.23	2/2058 (0.1%)
1	F	0.84	2/1450 (0.1%)	1.26	5/1946 (0.3%)
1	G	0.64	0/1427	1.10	0/1916
1	H	0.82	1/1449 (0.1%)	1.19	1/1946 (0.1%)
1	I	0.80	1/1520 (0.1%)	1.14	0/2043
1	J	0.70	0/1521	1.17	0/2043
1	K	0.60	0/1280	1.10	0/1719
1	L	0.65	0/1521	1.10	1/2043 (0.0%)
1	M	0.70	0/1434	1.13	1/1925 (0.1%)
1	N	0.76	0/1441	1.20	0/1936
1	O	0.86	1/1532 (0.1%)	1.21	2/2058 (0.1%)
1	P	0.70	0/1491	1.19	2/2000 (0.1%)
1	Q	0.77	0/1466	1.24	4/1966 (0.2%)
1	R	0.66	0/1396	1.12	2/1873 (0.1%)
All	All	0.72	6/26394 (0.0%)	1.16	20/35447 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	2
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	1
1	N	0	1
1	P	0	1
1	Q	0	1
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	94	ARG	C-O	-6.33	1.15	1.24
1	O	67	TYR	C-O	-5.38	1.17	1.24
1	E	87	LEU	C-O	-5.36	1.17	1.24
1	F	97	SER	CA-CB	-5.11	1.45	1.53
1	I	112	ILE	C-O	-5.06	1.18	1.24
1	H	160	ILE	C-O	-5.06	1.17	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	40	ILE	N-CA-C	-9.54	93.83	107.75
1	E	186	LYS	N-CA-C	7.57	119.17	111.07
1	F	116	LEU	CA-C-N	7.21	130.67	120.28
1	F	116	LEU	C-N-CA	7.21	130.67	120.28
1	M	65	THR	CA-CB-OG1	-6.97	99.15	109.60
1	L	50	GLU	N-CA-C	6.55	118.21	111.14
1	H	79	THR	CB-CA-C	5.82	122.15	109.99
1	O	43	LEU	N-CA-C	-5.68	105.66	112.59
1	F	95	TYR	CA-C-N	5.54	129.98	120.72
1	F	95	TYR	C-N-CA	5.54	129.98	120.72
1	F	14	LEU	N-CA-C	-5.39	104.82	111.40
1	Q	22	GLU	CB-CA-C	-5.22	102.45	110.81
1	O	117	CYS	N-CA-C	-5.21	105.66	112.23
1	P	126	ASP	CA-CB-CG	5.19	117.79	112.60
1	Q	23	ASN	CB-CA-C	-5.11	103.10	110.96
1	E	52	ASP	CA-CB-CG	5.09	117.69	112.60
1	R	168	LYS	CA-C-N	5.07	129.33	122.19
1	R	168	LYS	C-N-CA	5.07	129.33	122.19
1	Q	137	GLU	CA-C-N	5.02	127.51	120.28
1	Q	137	GLU	C-N-CA	5.02	127.51	120.28

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain
1	D	114	ARG	Sidechain
1	E	94	ARG	Sidechain
1	F	114	ARG	Sidechain
1	H	94	ARG	Sidechain
1	I	114	ARG	Sidechain
1	I	94	ARG	Sidechain
1	J	114	ARG	Sidechain
1	L	94	ARG	Sidechain
1	M	64	ARG	Sidechain
1	N	64	ARG	Sidechain
1	P	94	ARG	Sidechain
1	Q	114	ARG	Sidechain

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	1517	0	1528	23	0
1	B	1332	0	1280	12	0
1	C	1503	0	1513	23	0
1	D	1517	0	1529	27	2
1	E	1514	0	1523	30	1
1	F	1434	0	1453	44	0
1	G	1411	0	1428	21	0
1	H	1433	0	1444	31	0
1	I	1502	0	1511	31	1
1	J	1503	0	1512	21	0
1	K	1268	0	1230	16	0
1	L	1503	0	1513	23	0
1	M	1418	0	1429	16	2
1	N	1425	0	1433	47	0
1	O	1514	0	1523	34	0
1	P	1475	0	1488	25	0
1	Q	1450	0	1471	32	1
1	R	1380	0	1394	29	1
All	All	26099	0	26202	442	4

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 8.

All (442) 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:F:117:CYS:CB	1:O:117:CYS:SG	2.34	1.15
1:Q:84:LEU:HD13	1:Q:101:ILE:HD11	1.14	1.14
1:F:117:CYS:SG	1:O:117:CYS:CB	2.42	1.07
1:I:117:CYS:CB	1:N:117:CYS:SG	2.46	1.02
1:I:117:CYS:SG	1:N:117:CYS:CB	2.48	1.01
1:E:94:ARG:HG3	1:E:94:ARG:HH11	1.28	0.97
1:N:41:ASN:HB3	1:N:44:ALA:HB2	1.56	0.87
1:N:21:LEU:HD23	1:N:116:LEU:HD13	1.56	0.84
1:Q:84:LEU:CD1	1:Q:101:ILE:HD11	2.02	0.84
1:J:94:ARG:HG3	1:J:94:ARG:HH11	1.43	0.82
1:M:61:GLN:OE1	1:M:113:ASP:OD2	1.98	0.81
1:O:59:GLU:O	1:O:63:LYS:HG3	1.80	0.81
1:I:116:LEU:HG	1:I:120:LYS:HE3	1.64	0.80
1:H:61:GLN:NE2	1:H:113:ASP:OD2	2.16	0.79
1:Q:84:LEU:HD13	1:Q:101:ILE:CD1	2.07	0.77
1:D:172:THR:HG22	1:N:91:LEU:HG	1.64	0.77
1:F:12:SER:HB3	1:F:15:GLU:HB2	1.67	0.77
1:A:54:LEU:HD13	1:A:102:TYR:HE1	1.50	0.76
1:I:114:ARG:NH2	1:N:121:GLU:OE2	2.18	0.76
1:H:94:ARG:HG3	1:H:94:ARG:NH1	2.02	0.73
1:R:109:GLN:HE22	1:R:149:ARG:HH11	1.37	0.73
1:I:117:CYS:SG	1:N:117:CYS:SG	0.73	0.73
1:F:94:ARG:O	1:F:94:ARG:HG3	1.90	0.71
1:N:35:ILE:HG22	1:N:40:ILE:HD11	1.72	0.71
1:O:65:THR:OG1	1:O:109:GLN:NE2	2.24	0.71
1:K:172:THR:HG23	1:Q:89:ASN:HB3	1.72	0.71
1:K:172:THR:CG2	1:Q:89:ASN:HB3	2.21	0.70
1:P:62:ILE:HD13	1:P:101:ILE:HG23	1.73	0.69
1:H:147:LYS:HE3	1:L:158:GLU:HG3	1.74	0.69
1:I:188:LEU:HD23	1:I:188:LEU:C	2.18	0.69
1:Q:41:ASN:HB3	1:Q:44:ALA:HB2	1.74	0.68
1:F:65:THR:OG1	1:F:109:GLN:NE2	2.26	0.68
1:I:40:ILE:HD13	1:I:40:ILE:N	2.09	0.67
1:D:166:ASP:OD2	1:D:172:THR:HG23	1.94	0.67
1:J:55:SER:HB3	1:J:58:GLU:OE1	1.94	0.67
1:L:87:LEU:HD13	1:L:177:LEU:HD23	1.77	0.67
1:C:131:GLN:HE21	1:C:131:GLN:HA	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:ILE:O	1:N:195:ASN:ND2	2.28	0.66
1:F:61:GLN:NE2	1:F:113:ASP:OD2	2.29	0.66
1:K:104:ILE:O	1:K:108:ILE:HG12	1.96	0.66
1:R:163:TYR:CE1	1:R:171:GLN:HG3	2.31	0.66
1:M:60:MET:O	1:M:64:ARG:HG3	1.96	0.66
1:J:175:ASP:O	1:J:179:THR:HG23	1.96	0.66
1:O:179:THR:O	1:O:183:GLU:HG2	1.96	0.65
1:A:19:LYS:HG3	1:G:56:GLN:OE1	1.97	0.65
1:J:94:ARG:HG3	1:J:94:ARG:NH1	2.10	0.65
1:R:161:ASP:O	1:R:165:LYS:HG2	1.96	0.65
1:H:40:ILE:HD12	1:H:78:ASN:HD21	1.63	0.64
1:Q:29:TYR:O	1:Q:33:ASN:ND2	2.29	0.64
1:E:14:LEU:HD22	1:E:135:GLU:HG2	1.80	0.64
1:F:88:TYR:O	1:F:94:ARG:NH2	2.30	0.63
1:Q:124:ILE:O	1:Q:124:ILE:HG22	1.97	0.63
1:D:171:GLN:HG2	1:N:91:LEU:HD11	1.81	0.63
1:I:107:SER:HB3	1:I:188:LEU:HD12	1.81	0.63
1:F:117:CYS:SG	1:O:117:CYS:SG	0.63	0.62
1:G:56:GLN:CD	1:G:56:GLN:H	2.07	0.62
1:F:187:THR:HG23	1:F:190:SER:HB3	1.81	0.62
1:N:116:LEU:HG	1:N:120:LYS:HE3	1.79	0.62
1:O:64:ARG:HG2	1:O:64:ARG:HH11	1.65	0.61
1:H:35:ILE:HD11	1:H:72:TYR:HB3	1.82	0.61
1:D:171:GLN:HG2	1:N:91:LEU:CD1	2.30	0.61
1:D:172:THR:HG22	1:N:91:LEU:CG	2.30	0.61
1:M:62:ILE:HD13	1:M:101:ILE:HG23	1.82	0.61
1:N:61:GLN:OE1	1:N:113:ASP:OD2	2.18	0.61
1:E:180:TYR:HD1	1:E:181:MET:HE2	1.66	0.60
1:R:45:THR:CG2	1:R:88:TYR:CD2	2.84	0.60
1:C:29:TYR:O	1:C:33:ASN:ND2	2.29	0.60
1:D:172:THR:HG22	1:N:91:LEU:CD1	2.32	0.60
1:N:41:ASN:CB	1:N:44:ALA:HB2	2.30	0.60
1:I:21:LEU:HD23	1:I:116:LEU:HD13	1.84	0.60
1:P:35:ILE:HD11	1:P:72:TYR:HB3	1.84	0.60
1:E:94:ARG:HG3	1:E:94:ARG:NH1	2.06	0.59
1:F:88:TYR:CE2	1:F:94:ARG:HD2	2.37	0.59
1:M:41:ASN:HB3	1:M:44:ALA:HB2	1.83	0.59
1:A:22:GLU:OE1	1:A:22:GLU:HA	2.01	0.59
1:J:66:ILE:HD11	1:J:105:VAL:HG21	1.84	0.59
1:N:115:VAL:HG11	1:N:142:LEU:HA	1.84	0.58
1:O:41:ASN:HB3	1:O:44:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:114:ARG:O	1:O:114:ARG:HG2	2.01	0.58
1:J:56:GLN:HE22	1:P:19:LYS:HE3	1.68	0.58
1:C:42:PHE:HA	1:C:81:LYS:HE2	1.85	0.58
1:L:180:TYR:O	1:L:184:ASN:ND2	2.36	0.58
1:R:35:ILE:HD11	1:R:72:TYR:HB3	1.86	0.58
1:F:14:LEU:HD12	1:F:139:LEU:HD13	1.86	0.58
1:G:109:GLN:HE22	1:G:149:ARG:HH11	1.52	0.58
1:I:57:TYR:CE2	1:N:120:LYS:HG2	2.39	0.58
1:Q:74:LYS:O	1:Q:78:ASN:ND2	2.37	0.57
1:D:90:LYS:N	1:D:90:LYS:HD3	2.19	0.57
1:F:108:ILE:HD13	1:F:188:LEU:HD12	1.86	0.57
1:P:61:GLN:NE2	1:P:113:ASP:OD2	2.36	0.57
1:I:111:ASP:O	1:I:115:VAL:HG23	2.04	0.57
1:A:54:LEU:HD13	1:A:102:TYR:CE1	2.36	0.57
1:K:40:ILE:HD12	1:K:77:ILE:HD11	1.87	0.57
1:M:167:SER:O	1:M:170:ILE:HG12	2.06	0.56
1:A:100:PHE:O	1:A:105:VAL:HG23	2.05	0.56
1:R:163:TYR:CZ	1:R:171:GLN:HG3	2.40	0.56
1:N:59:GLU:O	1:N:63:LYS:HG3	2.05	0.56
1:F:120:LYS:HE2	1:O:57:TYR:CE1	2.40	0.56
1:I:35:ILE:HD11	1:I:72:TYR:O	2.06	0.56
1:N:82:GLU:O	1:N:86:THR:OG1	2.22	0.56
1:P:42:PHE:HA	1:P:81:LYS:HD2	1.87	0.56
1:N:34:GLU:O	1:N:38:GLN:NE2	2.39	0.55
1:H:107:SER:HB3	1:H:188:LEU:HD12	1.88	0.55
1:L:110:TYR:OH	1:L:114:ARG:NH1	2.39	0.55
1:P:161:ASP:O	1:P:165:LYS:HG2	2.06	0.55
1:P:59:GLU:OE2	1:P:63:LYS:NZ	2.29	0.55
1:B:16:THR:HA	1:B:19:LYS:HG2	1.89	0.55
1:C:134:LYS:HA	1:C:134:LYS:HE3	1.88	0.55
1:F:110:TYR:OH	1:O:121:GLU:HG3	2.06	0.55
1:A:61:GLN:NE2	1:A:113:ASP:OD2	2.39	0.55
1:A:61:GLN:O	1:A:64:ARG:HB2	2.07	0.55
1:F:90:LYS:HG2	1:F:93:HIS:HD2	1.72	0.55
1:R:156:LEU:O	1:R:160:ILE:HG12	2.07	0.54
1:D:52:ASP:OD1	1:D:52:ASP:N	2.40	0.54
1:O:162:ASP:OD2	1:O:180:TYR:OH	2.26	0.54
1:Q:167:SER:O	1:Q:170:ILE:HG12	2.07	0.54
1:D:131:GLN:HE22	1:D:135:GLU:CG	2.21	0.54
1:J:167:SER:O	1:J:170:ILE:HG12	2.07	0.54
1:R:104:ILE:O	1:R:108:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:ASN:HB3	1:L:44:ALA:HB2	1.90	0.54
1:N:62:ILE:HD13	1:N:101:ILE:HG23	1.88	0.54
1:E:54:LEU:HD13	1:E:102:TYR:HE1	1.72	0.54
1:M:21:LEU:HD11	1:M:142:LEU:HD11	1.90	0.54
1:R:61:GLN:HE21	1:R:109:GLN:HG3	1.73	0.54
1:J:56:GLN:HE22	1:P:19:LYS:CE	2.21	0.54
1:B:170:ILE:HG12	1:B:177:LEU:HD13	1.90	0.53
1:F:88:TYR:CD2	1:F:94:ARG:HD2	2.43	0.53
1:N:167:SER:O	1:N:170:ILE:HG12	2.09	0.53
1:F:119:ILE:CD1	1:F:138:LEU:HB3	2.39	0.53
1:N:90:LYS:NZ	1:N:175:ASP:OD1	2.41	0.53
1:O:54:LEU:HD13	1:O:102:TYR:HE1	1.73	0.53
1:J:94:ARG:HH11	1:J:94:ARG:CG	2.17	0.53
1:A:70:LEU:HD21	1:A:156:LEU:HG	1.90	0.53
1:C:188:LEU:HD12	1:C:188:LEU:N	2.24	0.53
1:N:56:GLN:CD	1:N:56:GLN:H	2.17	0.53
1:F:65:THR:O	1:F:69:SER:OG	2.25	0.52
1:L:94:ARG:O	1:L:97:SER:HB3	2.09	0.52
1:R:62:ILE:HD13	1:R:101:ILE:HG12	1.91	0.52
1:C:54:LEU:HD13	1:C:102:TYR:HE1	1.73	0.52
1:A:107:SER:HB3	1:A:188:LEU:HD22	1.91	0.52
1:D:130:THR:HG22	1:D:130:THR:O	2.09	0.52
1:R:155:LYS:O	1:R:155:LYS:HG3	2.10	0.52
1:A:35:ILE:HD11	1:A:72:TYR:HB3	1.92	0.52
1:H:94:ARG:HG3	1:H:94:ARG:HH11	1.72	0.52
1:J:46:PHE:O	1:J:49:ASP:HB3	2.10	0.52
1:O:67:TYR:HB3	1:O:72:TYR:CD1	2.45	0.52
1:N:156:LEU:O	1:N:160:ILE:HG12	2.10	0.52
1:P:65:THR:OG1	1:P:109:GLN:OE1	2.28	0.52
1:N:80:LEU:HA	1:N:83:ILE:HD12	1.91	0.51
1:C:131:GLN:HE21	1:C:131:GLN:CA	2.24	0.51
1:F:90:LYS:HG3	1:F:92:GLN:OE1	2.09	0.51
1:P:98:LYS:O	1:P:99:GLU:C	2.53	0.51
1:I:38:GLN:O	1:I:40:ILE:HD13	2.10	0.51
1:M:25:ASN:O	1:M:64:ARG:NH1	2.37	0.51
1:A:41:ASN:HB3	1:A:44:ALA:HB2	1.92	0.51
1:O:187:THR:O	1:O:190:SER:OG	2.29	0.51
1:R:21:LEU:HD21	1:R:142:LEU:HD21	1.93	0.51
1:G:40:ILE:HG23	1:G:40:ILE:O	2.11	0.51
1:A:18:ALA:O	1:A:22:GLU:HB2	2.11	0.51
1:A:165:LYS:O	1:A:165:LYS:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LYS:O	1:C:64:ARG:C	2.54	0.51
1:F:41:ASN:HB3	1:F:44:ALA:HB2	1.93	0.51
1:A:26:LYS:HD3	1:G:29:TYR:OH	2.11	0.51
1:I:121:GLU:HG3	1:N:110:TYR:OH	2.11	0.51
1:Q:94:ARG:HH11	1:Q:94:ARG:CG	2.22	0.51
1:H:32:ILE:HG21	1:H:60:MET:HE1	1.93	0.50
1:A:71:ASN:CG	1:A:71:ASN:O	2.54	0.50
1:D:61:GLN:O	1:D:109:GLN:HG3	2.12	0.50
1:H:32:ILE:HD13	1:H:60:MET:CE	2.40	0.50
1:H:47:LYS:HG3	1:H:54:LEU:HD23	1.92	0.50
1:I:135:GLU:N	1:Q:137:GLU:OE2	2.45	0.50
1:L:21:LEU:HD11	1:L:142:LEU:HD11	1.93	0.50
1:R:41:ASN:HB3	1:R:44:ALA:HB2	1.94	0.50
1:J:54:LEU:HD13	1:J:102:TYR:HE1	1.77	0.50
1:H:167:SER:O	1:H:170:ILE:HG12	2.12	0.50
1:N:99:GLU:O	1:N:103:GLN:HB3	2.11	0.50
1:F:35:ILE:HD11	1:F:72:TYR:HB3	1.92	0.50
1:K:171:GLN:OE1	1:Q:91:LEU:HD11	2.12	0.50
1:C:100:PHE:O	1:C:105:VAL:HG23	2.11	0.50
1:A:127:ASN:OD1	1:G:58:GLU:OE2	2.30	0.49
1:E:32:ILE:HG12	1:E:67:TYR:CD2	2.47	0.49
1:C:107:SER:HB3	1:C:188:LEU:HD23	1.94	0.49
1:E:134:LYS:HD2	1:G:137:GLU:HB2	1.94	0.49
1:I:188:LEU:HD23	1:I:188:LEU:O	2.12	0.49
1:K:166:ASP:HB2	1:Q:91:LEU:HD12	1.94	0.49
1:O:61:GLN:HA	1:O:64:ARG:HD2	1.94	0.49
1:R:62:ILE:CD1	1:R:101:ILE:HG12	2.41	0.49
1:G:173:ASN:OD1	1:G:175:ASP:HB2	2.11	0.49
1:M:80:LEU:O	1:M:84:LEU:HG	2.12	0.49
1:N:74:LYS:O	1:N:78:ASN:OD1	2.30	0.49
1:I:117:CYS:HG	1:N:117:CYS:CB	2.10	0.49
1:F:90:LYS:HE3	1:F:92:GLN:OE1	2.13	0.49
1:F:29:TYR:CZ	1:O:26:LYS:CD	2.96	0.49
1:I:88:TYR:CE2	1:I:94:ARG:HD3	2.48	0.49
1:N:35:ILE:CG2	1:N:40:ILE:HD11	2.43	0.49
1:H:163:TYR:HD1	1:H:170:ILE:HG22	1.78	0.48
1:F:88:TYR:CD2	1:F:94:ARG:CD	2.96	0.48
1:K:38:GLN:OE1	1:K:74:LYS:HD3	2.14	0.48
1:I:41:ASN:HB3	1:I:44:ALA:HB2	1.96	0.48
1:F:29:TYR:CZ	1:O:26:LYS:HD3	2.48	0.48
1:F:30:ILE:HG13	1:F:31:LYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:ILE:HG22	1:O:67:TYR:HD1	1.78	0.48
1:O:173:ASN:O	1:O:176:ALA:HB3	2.14	0.48
1:N:144:SER:O	1:N:148:THR:OG1	2.31	0.48
1:O:64:ARG:HG2	1:O:64:ARG:NH1	2.26	0.48
1:R:59:GLU:OE2	1:R:63:LYS:NZ	2.44	0.48
1:B:35:ILE:HD11	1:B:67:TYR:CD2	2.48	0.48
1:F:119:ILE:HD11	1:F:138:LEU:HB3	1.96	0.48
1:H:92:GLN:O	1:H:95:TYR:HE1	1.96	0.48
1:I:45:THR:HG21	1:I:85:GLU:HG2	1.95	0.48
1:O:17:ALA:O	1:O:21:LEU:HB2	2.14	0.48
1:R:137:GLU:HG3	1:R:138:LEU:N	2.29	0.48
1:F:112:ILE:HD13	1:F:146:LEU:HD23	1.94	0.48
1:O:67:TYR:HD1	1:O:67:TYR:N	2.10	0.48
1:R:109:GLN:HE22	1:R:149:ARG:NH1	2.07	0.48
1:N:21:LEU:HD22	1:N:142:LEU:HD11	1.94	0.48
1:L:40:ILE:HG13	1:L:78:ASN:HD21	1.78	0.47
1:O:125:LYS:HD2	1:O:130:THR:HG23	1.96	0.47
1:Q:115:VAL:O	1:Q:118:LEU:N	2.47	0.47
1:C:41:ASN:HB3	1:C:44:ALA:HB2	1.96	0.47
1:G:23:ASN:O	1:G:27:GLN:HG2	2.14	0.47
1:H:107:SER:HB3	1:H:188:LEU:CD1	2.43	0.47
1:O:67:TYR:N	1:O:67:TYR:CD1	2.81	0.47
1:L:125:LYS:HD3	1:L:130:THR:O	2.15	0.47
1:O:173:ASN:OD1	1:O:173:ASN:C	2.57	0.47
1:F:70:LEU:HD23	1:F:157:ASN:ND2	2.29	0.47
1:K:142:LEU:HG	1:K:146:LEU:HD12	1.96	0.47
1:O:183:GLU:O	1:O:186:LYS:NZ	2.40	0.47
1:P:115:VAL:HG12	1:P:119:ILE:HD12	1.95	0.47
1:B:146:LEU:O	1:B:150:GLN:HG2	2.14	0.47
1:D:63:LYS:O	1:D:67:TYR:HB2	2.13	0.47
1:D:171:GLN:CG	1:N:91:LEU:HD11	2.44	0.47
1:J:107:SER:HB2	1:J:188:LEU:HD13	1.97	0.47
1:D:171:GLN:HE22	1:E:90:LYS:NZ	2.13	0.47
1:H:41:ASN:HB3	1:H:44:ALA:HB2	1.96	0.47
1:I:47:LYS:NZ	1:I:59:GLU:OE2	2.45	0.47
1:I:47:LYS:CE	1:I:59:GLU:OE2	2.63	0.47
1:N:166:ASP:OD1	1:N:172:THR:HG22	2.14	0.47
1:O:111:ASP:O	1:O:115:VAL:HG23	2.15	0.47
1:P:42:PHE:CD2	1:P:43:LEU:HG	2.50	0.47
1:Q:170:ILE:HD12	1:Q:177:LEU:HA	1.95	0.47
1:B:59:GLU:HG2	1:B:63:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:THR:OG1	1:D:109:GLN:HG2	2.14	0.47
1:H:163:TYR:CE1	1:H:171:GLN:HA	2.50	0.47
1:E:32:ILE:HD11	1:E:64:ARG:HA	1.96	0.47
1:F:35:ILE:HG22	1:F:40:ILE:HD11	1.97	0.47
1:F:140:MET:HB3	1:F:140:MET:HE2	1.72	0.47
1:A:21:LEU:HA	1:A:24:GLN:HG2	1.97	0.47
1:D:74:LYS:HB3	1:E:172:THR:HG23	1.96	0.46
1:G:91:LEU:HD13	1:R:172:THR:CG2	2.45	0.46
1:H:95:TYR:O	1:H:99:GLU:N	2.41	0.46
1:C:107:SER:CB	1:C:188:LEU:HD23	2.45	0.46
1:F:41:ASN:CB	1:F:44:ALA:HB2	2.45	0.46
1:H:40:ILE:HD12	1:H:78:ASN:ND2	2.30	0.46
1:H:188:LEU:C	1:H:188:LEU:HD23	2.40	0.46
1:J:40:ILE:HD11	1:J:78:ASN:HD21	1.80	0.46
1:J:118:LEU:HB3	1:J:133:GLN:HE22	1.80	0.46
1:Q:88:TYR:O	1:Q:94:ARG:NH1	2.48	0.46
1:D:158:GLU:HG3	1:M:147:LYS:HE3	1.96	0.46
1:G:109:GLN:HE22	1:G:149:ARG:NH1	2.14	0.46
1:Q:124:ILE:O	1:Q:124:ILE:CG2	2.63	0.46
1:R:29:TYR:O	1:R:33:ASN:ND2	2.49	0.46
1:D:131:GLN:HE22	1:D:135:GLU:HG2	1.81	0.46
1:G:99:GLU:O	1:G:103:GLN:HB2	2.16	0.46
1:P:32:ILE:HD11	1:P:64:ARG:HA	1.97	0.46
1:F:70:LEU:HD23	1:F:157:ASN:HD21	1.81	0.46
1:J:105:VAL:HG22	1:J:152:PHE:CZ	2.50	0.46
1:N:194:ILE:O	1:N:195:ASN:CG	2.59	0.46
1:F:49:ASP:HB2	1:F:88:TYR:OH	2.16	0.46
1:G:61:GLN:NE2	1:G:113:ASP:OD2	2.48	0.46
1:H:170:ILE:HD12	1:H:177:LEU:HA	1.98	0.46
1:L:49:ASP:OD1	1:L:49:ASP:C	2.58	0.46
1:P:41:ASN:HB3	1:P:44:ALA:HB2	1.96	0.46
1:K:140:MET:SD	1:K:140:MET:C	2.98	0.46
1:N:32:ILE:HD13	1:N:60:MET:HE3	1.97	0.46
1:C:121:GLU:HG3	1:C:125:LYS:HE2	1.97	0.45
1:E:95:TYR:CG	1:E:96:THR:N	2.84	0.45
1:Q:183:GLU:O	1:Q:186:LYS:HG3	2.16	0.45
1:R:30:ILE:HG13	1:R:31:LYS:N	2.32	0.45
1:L:92:GLN:HE21	1:P:91:LEU:HD13	1.81	0.45
1:Q:134:LYS:O	1:Q:138:LEU:HB2	2.16	0.45
1:O:32:ILE:HG12	1:O:67:TYR:CD2	2.50	0.45
1:E:158:GLU:HG3	1:Q:147:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:121:GLU:HG2	1:P:133:GLN:NE2	2.32	0.45
1:Q:124:ILE:C	1:Q:125:LYS:HG2	2.41	0.45
1:E:21:LEU:HD23	1:E:116:LEU:HD13	1.98	0.45
1:H:81:LYS:O	1:H:85:GLU:HG3	2.16	0.45
1:E:30:ILE:HG13	1:E:31:LYS:N	2.32	0.45
1:G:91:LEU:HD22	1:R:166:ASP:HB2	1.98	0.45
1:K:73:GLU:O	1:K:77:ILE:HG23	2.17	0.45
1:E:70:LEU:HD21	1:E:156:LEU:HG	1.97	0.45
1:G:62:ILE:HD13	1:G:101:ILE:HG23	1.99	0.45
1:H:107:SER:CB	1:H:188:LEU:HD12	2.46	0.45
1:L:87:LEU:HD13	1:L:177:LEU:CD2	2.45	0.45
1:C:30:ILE:HG13	1:C:31:LYS:N	2.32	0.45
1:F:109:GLN:HE22	1:F:149:ARG:HH11	1.64	0.45
1:F:122:ALA:O	1:F:125:LYS:N	2.47	0.45
1:E:84:LEU:HD13	1:E:101:ILE:HD11	1.99	0.45
1:B:100:PHE:O	1:B:104:ILE:HG23	2.17	0.44
1:C:188:LEU:HD12	1:C:188:LEU:H	1.82	0.44
1:D:93:HIS:HE1	1:D:175:ASP:OD1	2.00	0.44
1:E:51:LYS:H	1:E:51:LYS:HG2	1.50	0.44
1:H:94:ARG:HH11	1:H:94:ARG:CG	2.29	0.44
1:I:188:LEU:C	1:I:188:LEU:CD2	2.86	0.44
1:N:35:ILE:HD11	1:N:72:TYR:HB3	1.98	0.44
1:G:187:THR:HG23	1:G:190:SER:HB3	1.99	0.44
1:I:18:ALA:HA	1:I:116:LEU:HD11	1.99	0.44
1:P:16:THR:O	1:P:16:THR:HG22	2.17	0.44
1:Q:148:THR:HA	1:Q:191:PHE:O	2.17	0.44
1:B:12:SER:HB3	1:B:15:GLU:HB2	2.00	0.44
1:B:12:SER:OG	1:B:13:LYS:N	2.50	0.44
1:E:42:PHE:CD2	1:E:43:LEU:HG	2.53	0.44
1:J:86:THR:HG22	1:J:174:VAL:HG23	1.98	0.44
1:A:180:TYR:CZ	1:A:184:ASN:ND2	2.86	0.44
1:L:14:LEU:HG	1:L:135:GLU:HG3	2.00	0.44
1:R:57:TYR:CZ	1:R:61:GLN:OE1	2.70	0.44
1:A:104:ILE:HD13	1:A:185:TYR:HB3	2.00	0.44
1:C:96:THR:HG22	1:C:182:LYS:HD3	1.99	0.44
1:E:47:LYS:C	1:E:49:ASP:H	2.25	0.44
1:F:144:SER:O	1:F:148:THR:OG1	2.26	0.43
1:G:103:GLN:O	1:G:107:SER:OG	2.24	0.43
1:P:67:TYR:HB3	1:P:72:TYR:CD1	2.53	0.43
1:E:84:LEU:HD21	1:E:100:PHE:CD2	2.53	0.43
1:G:35:ILE:HD11	1:G:72:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:ILE:CD1	1:N:101:ILE:HG23	2.48	0.43
1:R:139:LEU:O	1:R:139:LEU:HD12	2.19	0.43
1:N:115:VAL:HG11	1:N:142:LEU:CA	2.48	0.43
1:C:61:GLN:HE22	1:C:64:ARG:HE	1.66	0.43
1:M:81:LYS:O	1:M:85:GLU:HG3	2.18	0.43
1:B:104:ILE:O	1:B:108:ILE:HG13	2.18	0.43
1:E:12:SER:O	1:E:16:THR:OG1	2.36	0.43
1:I:14:LEU:HD23	1:I:139:LEU:HD21	2.01	0.43
1:O:128:LEU:HB2	1:O:130:THR:HG22	1.99	0.43
1:R:101:ILE:HG23	1:R:102:TYR:CD2	2.54	0.43
1:C:88:TYR:CE1	1:C:94:ARG:NH1	2.86	0.43
1:Q:94:ARG:CG	1:Q:94:ARG:NH1	2.80	0.43
1:C:62:ILE:HD13	1:C:101:ILE:HD11	2.00	0.43
1:I:103:GLN:OE1	1:I:103:GLN:HA	2.18	0.43
1:J:173:ASN:O	1:J:176:ALA:HB3	2.19	0.43
1:L:70:LEU:HD21	1:L:156:LEU:HG	2.00	0.43
1:A:32:ILE:HG12	1:A:67:TYR:CD2	2.54	0.43
1:C:118:LEU:HD22	1:C:133:GLN:HE22	1.84	0.43
1:F:108:ILE:CD1	1:F:148:THR:HG22	2.48	0.43
1:L:116:LEU:HG	1:L:120:LYS:HE2	2.01	0.43
1:D:32:ILE:HG12	1:D:67:TYR:CD2	2.54	0.43
1:D:89:ASN:C	1:D:90:LYS:HD3	2.44	0.43
1:L:21:LEU:HD11	1:L:142:LEU:CD1	2.49	0.43
1:L:87:LEU:CD1	1:L:177:LEU:HD23	2.48	0.43
1:M:32:ILE:HD11	1:M:64:ARG:HA	2.01	0.43
1:P:30:ILE:HG13	1:P:31:LYS:N	2.33	0.43
1:Q:189:ASP:OD1	1:Q:192:LYS:HE2	2.19	0.43
1:R:95:TYR:CZ	1:R:96:THR:HG23	2.53	0.43
1:H:32:ILE:HD13	1:H:60:MET:HE3	2.01	0.42
1:L:120:LYS:O	1:L:124:ILE:HG23	2.18	0.42
1:G:74:LYS:O	1:G:75:GLN:C	2.63	0.42
1:R:166:ASP:OD1	1:R:169:ASN:HA	2.19	0.42
1:B:28:GLU:O	1:B:32:ILE:HD12	2.19	0.42
1:B:121:GLU:O	1:B:125:LYS:HG3	2.19	0.42
1:H:99:GLU:O	1:H:103:GLN:HB2	2.19	0.42
1:H:194:ILE:O	1:H:195:ASN:CG	2.62	0.42
1:J:45:THR:HG23	1:J:46:PHE:CD2	2.54	0.42
1:K:35:ILE:CG2	1:K:40:ILE:HD11	2.49	0.42
1:G:125:LYS:O	1:G:125:LYS:HG3	2.20	0.42
1:L:27:GLN:NE2	1:Q:74:LYS:HE2	2.35	0.42
1:N:41:ASN:O	1:N:42:PHE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:163:TYR:HA	1:P:170:ILE:CG2	2.49	0.42
1:E:180:TYR:HD1	1:E:181:MET:CE	2.31	0.42
1:F:40:ILE:O	1:F:40:ILE:HG13	2.20	0.42
1:H:119:ILE:O	1:H:122:ALA:HB3	2.18	0.42
1:H:194:ILE:HB	1:L:155:LYS:HD2	2.00	0.42
1:L:42:PHE:CD2	1:L:43:LEU:HG	2.55	0.42
1:M:170:ILE:HD12	1:M:177:LEU:HA	2.00	0.42
1:E:61:GLN:O	1:E:109:GLN:HG2	2.20	0.42
1:E:159:THR:HG23	1:E:181:MET:HE1	2.01	0.42
1:F:57:TYR:CZ	1:F:61:GLN:HG3	2.54	0.42
1:H:170:ILE:HG23	1:H:177:LEU:HD13	2.00	0.42
1:I:127:ASN:OD1	1:N:58:GLU:OE1	2.38	0.42
1:C:61:GLN:NE2	1:C:64:ARG:HE	2.18	0.42
1:E:156:LEU:O	1:E:159:THR:HB	2.19	0.42
1:L:78:ASN:HD22	1:L:78:ASN:HA	1.76	0.42
1:L:163:TYR:CE1	1:L:171:GLN:HA	2.54	0.42
1:C:14:LEU:HD23	1:C:14:LEU:HA	1.95	0.42
1:D:26:LYS:O	1:D:30:ILE:HG12	2.20	0.42
1:F:61:GLN:O	1:F:109:GLN:HG2	2.20	0.42
1:N:66:ILE:HD12	1:N:80:LEU:CD2	2.50	0.42
1:A:69:SER:HB3	1:A:153:ALA:HA	2.02	0.41
1:K:170:ILE:HD11	1:K:180:TYR:HB2	2.02	0.41
1:O:108:ILE:HG13	1:O:188:LEU:HD13	2.02	0.41
1:P:40:ILE:HG23	1:P:40:ILE:O	2.20	0.41
1:M:66:ILE:HG22	1:M:67:TYR:HD1	1.85	0.41
1:Q:17:ALA:O	1:Q:21:LEU:HB2	2.20	0.41
1:D:95:TYR:OH	1:D:182:LYS:HD3	2.20	0.41
1:D:130:THR:O	1:D:130:THR:CG2	2.68	0.41
1:F:65:THR:OG1	1:F:109:GLN:HB2	2.21	0.41
1:J:62:ILE:HD13	1:J:101:ILE:HG23	2.02	0.41
1:O:35:ILE:HD11	1:O:72:TYR:O	2.20	0.41
1:A:116:LEU:HG	1:A:120:LYS:HE3	2.02	0.41
1:D:193:PRO:O	1:D:194:ILE:C	2.63	0.41
1:K:87:LEU:HD11	1:K:177:LEU:HG	2.02	0.41
1:O:116:LEU:HD11	1:O:120:LYS:HE3	2.03	0.41
1:Q:65:THR:OG1	1:Q:109:GLN:OE1	2.34	0.41
1:R:158:GLU:O	1:R:159:THR:C	2.63	0.41
1:A:41:ASN:HD22	1:A:41:ASN:HA	1.67	0.41
1:E:57:TYR:O	1:E:61:GLN:HG2	2.20	0.41
1:K:163:TYR:HA	1:K:170:ILE:HG22	2.02	0.41
1:R:93:HIS:ND1	1:R:178:ALA:CB	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:TYR:O	1:E:94:ARG:NH1	2.54	0.41
1:P:47:LYS:HE3	1:P:47:LYS:HB3	1.34	0.41
1:P:66:ILE:HD12	1:P:80:LEU:HD21	2.02	0.41
1:G:66:ILE:HD12	1:G:80:LEU:CD2	2.51	0.41
1:I:47:LYS:HE3	1:I:59:GLU:OE2	2.21	0.41
1:J:64:ARG:O	1:J:68:SER:OG	2.37	0.41
1:N:30:ILE:O	1:N:30:ILE:HG13	2.21	0.41
1:F:61:GLN:NE2	1:F:109:GLN:HG3	2.36	0.41
1:I:166:ASP:OD1	1:I:169:ASN:HA	2.21	0.41
1:N:71:ASN:O	1:N:71:ASN:CG	2.64	0.41
1:N:155:LYS:NZ	1:N:184:ASN:OD1	2.54	0.41
1:Q:138:LEU:HD12	1:Q:138:LEU:HA	1.81	0.41
1:Q:166:ASP:OD1	1:Q:171:GLN:HB3	2.20	0.41
1:F:90:LYS:HG2	1:F:93:HIS:CD2	2.53	0.41
1:H:160:ILE:O	1:H:160:ILE:CG2	2.69	0.41
1:I:56:GLN:H	1:I:56:GLN:CD	2.29	0.41
1:M:45:THR:CG2	1:M:88:TYR:CD1	3.03	0.41
1:M:170:ILE:HD13	1:M:170:ILE:HA	1.86	0.41
1:P:124:ILE:HD13	1:P:124:ILE:N	2.36	0.41
1:D:156:LEU:O	1:D:159:THR:N	2.53	0.41
1:J:35:ILE:HD11	1:J:72:TYR:HB3	2.02	0.41
1:P:173:ASN:OD1	1:P:173:ASN:C	2.64	0.41
1:Q:156:LEU:HA	1:Q:185:TYR:OH	2.21	0.41
1:D:78:ASN:HD21	1:E:172:THR:HG22	1.85	0.40
1:E:49:ASP:OD1	1:E:51:LYS:CG	2.69	0.40
1:E:65:THR:OG1	1:E:109:GLN:NE2	2.45	0.40
1:R:69:SER:HA	1:R:153:ALA:HB1	2.03	0.40
1:I:32:ILE:HD11	1:I:64:ARG:HA	2.03	0.40
1:M:47:LYS:CE	1:M:59:GLU:OE2	2.69	0.40
1:H:105:VAL:HG22	1:H:152:PHE:CZ	2.55	0.40
1:K:41:ASN:HB3	1:K:44:ALA:HB2	2.03	0.40
1:Q:16:THR:O	1:Q:20:ASN:ND2	2.54	0.40
1:B:152:PHE:CD1	1:B:152:PHE:C	2.98	0.40
1:K:99:GLU:O	1:K:103:GLN:HB2	2.21	0.40
1:O:61:GLN:O	1:O:109:GLN:HG2	2.21	0.40
1:C:162:ASP:C	1:C:170:ILE:HD11	2.46	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:CYS:SG	1:M:117:CYS:SG[1_556]	1.65	0.55
1:E:127:ASN:OD1	1:Q:58:GLU:OE1[1_554]	2.06	0.14
1:I:90:LYS:NZ	1:R:164:ASN:OD1[1_556]	2.12	0.08
1:D:127:ASN:OD1	1:M:58:GLU:OE2[1_556]	2.18	0.02

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	181/194 (93%)	170 (94%)	11 (6%)	0	100	100
1	B	166/194 (86%)	161 (97%)	5 (3%)	0	100	100
1	C	179/194 (92%)	169 (94%)	10 (6%)	0	100	100
1	D	181/194 (93%)	173 (96%)	8 (4%)	0	100	100
1	E	181/194 (93%)	174 (96%)	7 (4%)	0	100	100
1	F	169/194 (87%)	163 (96%)	6 (4%)	0	100	100
1	G	166/194 (86%)	158 (95%)	8 (5%)	0	100	100
1	H	169/194 (87%)	164 (97%)	5 (3%)	0	100	100
1	I	179/194 (92%)	173 (97%)	6 (3%)	0	100	100
1	J	179/194 (92%)	168 (94%)	11 (6%)	0	100	100
1	K	154/194 (79%)	148 (96%)	6 (4%)	0	100	100
1	L	179/194 (92%)	176 (98%)	3 (2%)	0	100	100
1	M	167/194 (86%)	157 (94%)	10 (6%)	0	100	100
1	N	168/194 (87%)	157 (94%)	11 (6%)	0	100	100
1	O	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
1	P	174/194 (90%)	164 (94%)	10 (6%)	0	100	100
1	Q	171/194 (88%)	162 (95%)	9 (5%)	0	100	100
1	R	162/194 (84%)	157 (97%)	5 (3%)	0	100	100
All	All	3106/3492 (89%)	2965 (96%)	141 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	172/179 (96%)	158 (92%)	14 (8%)	11	33
1	B	136/179 (76%)	128 (94%)	8 (6%)	18	48
1	C	170/179 (95%)	159 (94%)	11 (6%)	15	44
1	D	172/179 (96%)	160 (93%)	12 (7%)	14	40
1	E	171/179 (96%)	155 (91%)	16 (9%)	8	26
1	F	162/179 (90%)	148 (91%)	14 (9%)	10	30
1	G	159/179 (89%)	155 (98%)	4 (2%)	42	74
1	H	162/179 (90%)	148 (91%)	14 (9%)	10	30
1	I	170/179 (95%)	159 (94%)	11 (6%)	15	44
1	J	170/179 (95%)	163 (96%)	7 (4%)	27	61
1	K	135/179 (75%)	128 (95%)	7 (5%)	21	52
1	L	170/179 (95%)	155 (91%)	15 (9%)	9	29
1	M	160/179 (89%)	150 (94%)	10 (6%)	16	45
1	N	161/179 (90%)	142 (88%)	19 (12%)	5	17
1	O	171/179 (96%)	155 (91%)	16 (9%)	8	26
1	P	167/179 (93%)	150 (90%)	17 (10%)	7	23
1	Q	164/179 (92%)	152 (93%)	12 (7%)	13	38
1	R	156/179 (87%)	145 (93%)	11 (7%)	13	40
All	All	2928/3222 (91%)	2710 (93%)	218 (7%)	13	38

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	22	GLU
1	A	52	ASP

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Mol	Chain	Res	Type
1	A	55	SER
1	A	90	LYS
1	A	119	ILE
1	A	125	LYS
1	A	134	LYS
1	A	135	GLU
1	A	170	ILE
1	A	172	THR
1	A	188	LEU
1	A	189	ASP
1	A	194	ILE
1	B	16	THR
1	B	20	ASN
1	B	32	ILE
1	B	35	ILE
1	B	49	ASP
1	B	52	ASP
1	B	74	LYS
1	B	99	GLU
1	C	13	LYS
1	C	26	LYS
1	C	35	ILE
1	C	52	ASP
1	C	71	ASN
1	C	89	ASN
1	C	90	LYS
1	C	101	ILE
1	C	131	GLN
1	C	134	LYS
1	C	144	SER
1	D	35	ILE
1	D	50	GLU
1	D	52	ASP
1	D	90	LYS
1	D	92	GLN
1	D	114	ARG
1	D	137	GLU
1	D	158	GLU
1	D	171	GLN
1	D	188	LEU
1	D	189	ASP
1	D	194	ILE

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Mol	Chain	Res	Type
1	E	16	THR
1	E	19	LYS
1	E	34	GLU
1	E	51	LYS
1	E	52	ASP
1	E	55	SER
1	E	56	GLN
1	E	91	LEU
1	E	94	ARG
1	E	96	THR
1	E	131	GLN
1	E	145	SER
1	E	156	LEU
1	E	170	ILE
1	E	172	THR
1	E	187	THR
1	F	26	LYS
1	F	30	ILE
1	F	45	THR
1	F	51	LYS
1	F	94	ARG
1	F	99	GLU
1	F	117	CYS
1	F	139	LEU
1	F	140	MET
1	F	142	LEU
1	F	179	THR
1	F	187	THR
1	F	188	LEU
1	F	194	ILE
1	G	65	THR
1	G	125	LYS
1	G	161	ASP
1	G	194	ILE
1	H	14	LEU
1	H	16	THR
1	H	38	GLN
1	H	45	THR
1	H	50	GLU
1	H	68	SER
1	H	75	GLN
1	H	90	LYS

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Mol	Chain	Res	Type
1	H	94	ARG
1	H	101	ILE
1	H	154	LYS
1	H	160	ILE
1	H	168	LYS
1	H	170	ILE
1	I	14	LEU
1	I	19	LYS
1	I	33	ASN
1	I	40	ILE
1	I	52	ASP
1	I	103	GLN
1	I	117	CYS
1	I	138	LEU
1	I	167	SER
1	I	179	THR
1	I	186	LYS
1	J	40	ILE
1	J	41	ASN
1	J	52	ASP
1	J	56	GLN
1	J	94	ARG
1	J	99	GLU
1	J	143	ASP
1	K	77	ILE
1	K	84	LEU
1	K	124	ILE
1	K	135	GLU
1	K	137	GLU
1	K	168	LYS
1	K	170	ILE
1	L	50	GLU
1	L	51	LYS
1	L	52	ASP
1	L	65	THR
1	L	76	LYS
1	L	87	LEU
1	L	101	ILE
1	L	104	ILE
1	L	124	ILE
1	L	134	LYS
1	L	137	GLU

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Mol	Chain	Res	Type
1	L	146	LEU
1	L	169	ASN
1	L	172	THR
1	L	182	LYS
1	M	16	THR
1	M	19	LYS
1	M	51	LYS
1	M	66	ILE
1	M	118	LEU
1	M	119	ILE
1	M	160	ILE
1	M	166	ASP
1	M	170	ILE
1	M	187	THR
1	N	14	LEU
1	N	16	THR
1	N	19	LYS
1	N	23	ASN
1	N	30	ILE
1	N	38	GLN
1	N	54	LEU
1	N	55	SER
1	N	65	THR
1	N	101	ILE
1	N	115	VAL
1	N	117	CYS
1	N	135	GLU
1	N	136	SER
1	N	141	ASN
1	N	155	LYS
1	N	170	ILE
1	N	172	THR
1	N	175	ASP
1	O	12	SER
1	O	25	ASN
1	O	35	ILE
1	O	52	ASP
1	O	55	SER
1	O	63	LYS
1	O	73	GLU
1	O	104	ILE
1	O	117	CYS

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Mol	Chain	Res	Type
1	O	134	LYS
1	O	135	GLU
1	O	173	ASN
1	O	174	VAL
1	O	186	LYS
1	O	188	LEU
1	O	190	SER
1	P	13	LYS
1	P	21	LEU
1	P	35	ILE
1	P	45	THR
1	P	47	LYS
1	P	51	LYS
1	P	56	GLN
1	P	92	GLN
1	P	103	GLN
1	P	114	ARG
1	P	121	GLU
1	P	124	ILE
1	P	154	LYS
1	P	165	LYS
1	P	170	ILE
1	P	183	GLU
1	P	186	LYS
1	Q	21	LEU
1	Q	35	ILE
1	Q	40	ILE
1	Q	90	LYS
1	Q	92	GLN
1	Q	94	ARG
1	Q	125	LYS
1	Q	138	LEU
1	Q	139	LEU
1	Q	142	LEU
1	Q	145	SER
1	Q	170	ILE
1	R	19	LYS
1	R	21	LEU
1	R	23	ASN
1	R	103	GLN
1	R	124	ILE
1	R	137	GLU

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Mol	Chain	Res	Type
1	R	139	LEU
1	R	142	LEU
1	R	155	LYS
1	R	167	SER
1	R	170	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	41	ASN
1	A	127	ASN
1	A	131	GLN
1	A	133	GLN
1	A	141	ASN
1	B	24	GLN
1	B	78	ASN
1	B	92	GLN
1	B	164	ASN
1	B	169	ASN
1	C	61	GLN
1	C	127	ASN
1	C	131	GLN
1	C	133	GLN
1	D	27	GLN
1	D	56	GLN
1	D	93	HIS
1	D	131	GLN
1	D	133	GLN
1	D	169	ASN
1	D	171	GLN
1	E	56	GLN
1	E	61	GLN
1	E	92	GLN
1	E	109	GLN
1	E	164	ASN
1	F	109	GLN
1	F	150	GLN
1	F	169	ASN
1	G	53	ASN
1	G	61	GLN
1	G	103	GLN

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Mol	Chain	Res	Type
1	G	109	GLN
1	G	151	ASN
1	H	24	GLN
1	H	38	GLN
1	H	53	ASN
1	H	78	ASN
1	H	151	ASN
1	H	157	ASN
1	I	33	ASN
1	I	53	ASN
1	I	89	ASN
1	I	127	ASN
1	I	129	HIS
1	I	169	ASN
1	J	20	ASN
1	J	56	GLN
1	J	78	ASN
1	J	133	GLN
1	J	184	ASN
1	K	23	ASN
1	K	33	ASN
1	K	61	GLN
1	L	23	ASN
1	L	27	GLN
1	L	33	ASN
1	L	41	ASN
1	L	78	ASN
1	L	89	ASN
1	L	129	HIS
1	L	151	ASN
1	L	169	ASN
1	M	27	GLN
1	M	61	GLN
1	M	78	ASN
1	M	89	ASN
1	M	164	ASN
1	N	27	GLN
1	N	33	ASN
1	N	41	ASN
1	N	53	ASN
1	N	56	GLN
1	N	78	ASN

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Mol	Chain	Res	Type
1	N	93	HIS
1	N	141	ASN
1	N	151	ASN
1	N	195	ASN
1	O	41	ASN
1	O	56	GLN
1	O	93	HIS
1	O	109	GLN
1	O	127	ASN
1	O	131	GLN
1	O	141	ASN
1	P	23	ASN
1	P	78	ASN
1	P	92	GLN
1	P	93	HIS
1	P	103	GLN
1	P	133	GLN
1	P	184	ASN
1	Q	20	ASN
1	Q	41	ASN
1	Q	93	HIS
1	Q	150	GLN
1	Q	184	ASN
1	R	109	GLN
1	R	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	183/194 (94%)	-0.16	1 (0%) 87 83	13, 25, 48, 57	0
1	B	170/194 (87%)	1.41	41 (24%) 2 2	55, 75, 89, 102	0
1	C	181/194 (93%)	0.28	6 (3%) 49 40	19, 41, 65, 84	0
1	D	183/194 (94%)	-0.05	2 (1%) 78 71	14, 28, 52, 67	0
1	E	183/194 (94%)	-0.17	0 100 100	12, 25, 46, 55	0
1	F	173/194 (89%)	-0.13	1 (0%) 85 81	13, 24, 46, 63	0
1	G	170/194 (87%)	-0.19	1 (0%) 85 81	12, 22, 42, 66	0
1	H	173/194 (89%)	0.03	2 (1%) 76 69	14, 28, 52, 87	0
1	I	181/194 (93%)	-0.12	1 (0%) 85 81	11, 24, 49, 66	0
1	J	181/194 (93%)	-0.23	0 100 100	9, 22, 45, 58	0
1	K	158/194 (81%)	1.02	25 (15%) 5 4	48, 65, 87, 104	0
1	L	181/194 (93%)	-0.23	0 100 100	9, 22, 39, 52	0
1	M	171/194 (88%)	0.01	3 (1%) 67 59	16, 27, 50, 71	0
1	N	172/194 (88%)	0.04	2 (1%) 76 69	14, 26, 51, 60	0
1	O	183/194 (94%)	-0.15	0 100 100	10, 27, 46, 63	0
1	P	178/194 (91%)	-0.10	4 (2%) 62 53	11, 22, 46, 73	0
1	Q	175/194 (90%)	-0.14	2 (1%) 78 71	12, 24, 42, 58	0
1	R	166/194 (85%)	0.05	3 (1%) 67 59	19, 32, 54, 67	0
All	All	3162/3492 (90%)	0.05	94 (2%) 52 43	9, 28, 72, 104	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	ASP	5.7
1	B	136	SER	4.8
1	P	195	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	56	GLN	4.5
1	B	42	PHE	4.4
1	B	41	ASN	4.0
1	B	161	ASP	3.9
1	B	179	THR	3.9
1	K	96	THR	3.6
1	B	143	ASP	3.5
1	C	136	SER	3.4
1	B	141	ASN	3.4
1	D	194	ILE	3.4
1	K	187	THR	3.4
1	N	14	LEU	3.3
1	C	13	LYS	3.2
1	B	48	ALA	3.1
1	B	157	ASN	3.1
1	C	132	ASN	3.1
1	Q	134	LYS	3.0
1	C	193	PRO	3.0
1	K	30	ILE	3.0
1	B	167	SER	3.0
1	B	112	ILE	2.9
1	B	12	SER	2.9
1	K	110	TYR	2.9
1	B	21	LEU	2.9
1	B	57	TYR	2.8
1	B	168	LYS	2.8
1	B	103	GLN	2.8
1	M	135	GLU	2.8
1	P	39	GLY	2.8
1	B	115	VAL	2.7
1	G	14	LEU	2.7
1	B	40	ILE	2.7
1	K	104	ILE	2.7
1	B	74	LYS	2.7
1	B	110	TYR	2.7
1	B	135	GLU	2.7
1	K	50	GLU	2.7
1	B	124	ILE	2.6
1	B	145	SER	2.6
1	I	194	ILE	2.6
1	K	51	LYS	2.5
1	K	91	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	122	ALA	2.5
1	B	140	MET	2.5
1	B	35	ILE	2.5
1	K	175	ASP	2.4
1	K	179	THR	2.4
1	B	126	ASP	2.4
1	P	134	LYS	2.4
1	K	135	GLU	2.3
1	B	91	LEU	2.3
1	Q	12	SER	2.3
1	D	110	TYR	2.3
1	B	174	VAL	2.3
1	B	54	LEU	2.3
1	K	138	LEU	2.3
1	K	66	ILE	2.3
1	K	57	TYR	2.3
1	B	14	LEU	2.2
1	B	47	LYS	2.2
1	K	118	LEU	2.2
1	K	26	LYS	2.2
1	B	51	LYS	2.2
1	B	43	LEU	2.2
1	N	135	GLU	2.2
1	B	75	GLN	2.1
1	K	38	GLN	2.1
1	K	92	GLN	2.1
1	K	48	ALA	2.1
1	B	93	HIS	2.1
1	K	120	LYS	2.1
1	K	188	LEU	2.1
1	K	45	THR	2.1
1	B	119	ILE	2.1
1	C	134	LYS	2.1
1	H	126	ASP	2.1
1	B	30	ILE	2.1
1	K	95	TYR	2.1
1	F	12	SER	2.0
1	H	125	LYS	2.0
1	M	125	LYS	2.0
1	B	116	LEU	2.0
1	B	138	LEU	2.0
1	B	18	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	189	ASP	2.0
1	R	18	ALA	2.0
1	P	12	SER	2.0
1	R	136	SER	2.0
1	K	124	ILE	2.0
1	A	22	GLU	2.0
1	M	189	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.