



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 06:07 PM EDT

PDB ID : 35UH / pdb_000035uh
Title : Crystal structure of TFPI K2 domain in complex with TFPI-23 Fab fragment
Authors : Juo, Z.S.; Bard, J.; Mosyak, L.
Deposited on : 2026-05-18
Resolution : 3.11 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

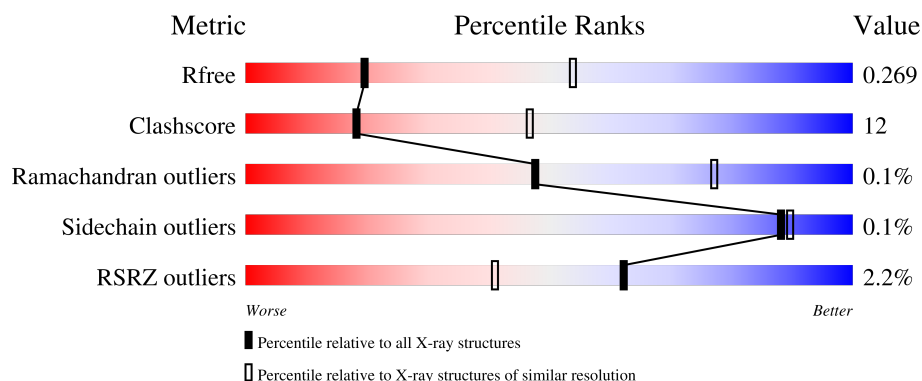
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> % 78% 17% . </div> </div>
1	D	223	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between;"> 80% 15% 5% </div> </div>
1	G	223	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 3% 71% 24% 5% </div> </div>
1	J	223	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> 3% 71% 24% 5% </div> </div>
1	M	223	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between;"> % 36% 18% 46% </div> </div>

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Mol	Chain	Length	Quality of chain
1	P	223	
2	B	218	
2	E	218	
2	H	218	
2	K	218	
2	N	218	
2	Q	218	
3	C	71	
3	F	71	
3	I	71	
3	L	71	
3	O	71	
3	R	71	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18693 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 TFPI-23-Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1566	989	260	310	7			
1	D	212	Total	C	N	O	S	0	0	0
			1560	986	259	308	7			
1	G	212	Total	C	N	O	S	0	0	0
			1560	986	259	308	7			
1	J	212	Total	C	N	O	S	0	0	0
			1560	986	259	308	7			
1	M	120	Total	C	N	O	S	0	0	0
			887	556	150	176	5			
1	P	120	Total	C	N	O	S	0	0	0
			887	556	150	176	5			

- Molecule 2 is a protein called TFPI-23-Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1578	983	265	326	4			
2	E	216	Total	C	N	O	S	0	0	0
			1587	988	266	329	4			
2	H	212	Total	C	N	O	S	0	0	0
			1558	972	262	320	4			
2	K	212	Total	C	N	O	S	0	0	0
			1558	972	262	320	4			
2	N	113	Total	C	N	O	S	0	0	0
			810	500	138	170	2			
2	Q	113	Total	C	N	O	S	0	0	0
			810	500	138	170	2			

- Molecule 3 is a protein called Tissue factor pathway inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			
3	F	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			
3	I	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			
3	L	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			
3	O	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			
3	R	56	Total	C	N	O	S	0	0	0
			462	288	77	90	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	151	GLY	-	expression tag	UNP Q2PFV4
C	152	GLY	-	expression tag	UNP Q2PFV4
C	153	SER	-	expression tag	UNP Q2PFV4
C	154	GLY	-	expression tag	UNP Q2PFV4
C	155	GLY	-	expression tag	UNP Q2PFV4
C	156	GLY	-	expression tag	UNP Q2PFV4
C	157	LEU	-	expression tag	UNP Q2PFV4
C	158	ASN	-	expression tag	UNP Q2PFV4
F	151	GLY	-	expression tag	UNP Q2PFV4
F	152	GLY	-	expression tag	UNP Q2PFV4
F	153	SER	-	expression tag	UNP Q2PFV4
F	154	GLY	-	expression tag	UNP Q2PFV4
F	155	GLY	-	expression tag	UNP Q2PFV4
F	156	GLY	-	expression tag	UNP Q2PFV4
F	157	LEU	-	expression tag	UNP Q2PFV4
F	158	ASN	-	expression tag	UNP Q2PFV4
I	151	GLY	-	expression tag	UNP Q2PFV4
I	152	GLY	-	expression tag	UNP Q2PFV4
I	153	SER	-	expression tag	UNP Q2PFV4
I	154	GLY	-	expression tag	UNP Q2PFV4
I	155	GLY	-	expression tag	UNP Q2PFV4
I	156	GLY	-	expression tag	UNP Q2PFV4
I	157	LEU	-	expression tag	UNP Q2PFV4
I	158	ASN	-	expression tag	UNP Q2PFV4
L	151	GLY	-	expression tag	UNP Q2PFV4
L	152	GLY	-	expression tag	UNP Q2PFV4
L	153	SER	-	expression tag	UNP Q2PFV4
L	154	GLY	-	expression tag	UNP Q2PFV4

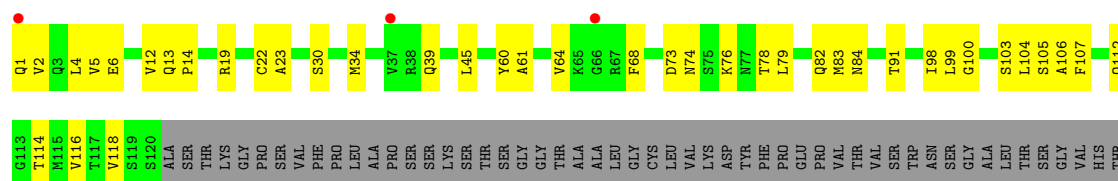
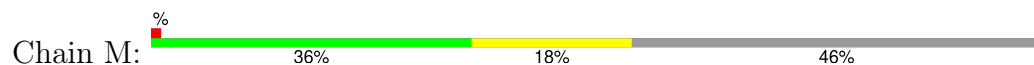
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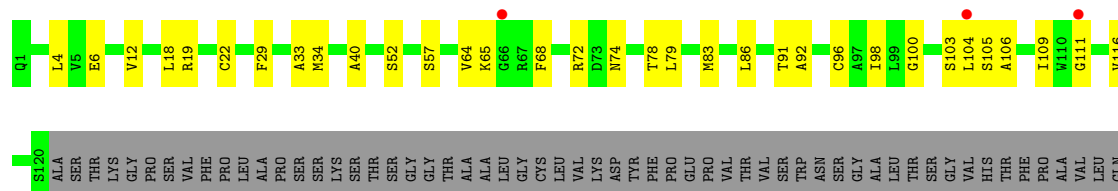
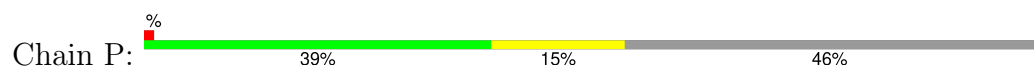
Chain	Residue	Modelled	Actual	Comment	Reference
L	155	GLY	-	expression tag	UNP Q2PFV4
L	156	GLY	-	expression tag	UNP Q2PFV4
L	157	LEU	-	expression tag	UNP Q2PFV4
L	158	ASN	-	expression tag	UNP Q2PFV4
O	151	GLY	-	expression tag	UNP Q2PFV4
O	152	GLY	-	expression tag	UNP Q2PFV4
O	153	SER	-	expression tag	UNP Q2PFV4
O	154	GLY	-	expression tag	UNP Q2PFV4
O	155	GLY	-	expression tag	UNP Q2PFV4
O	156	GLY	-	expression tag	UNP Q2PFV4
O	157	LEU	-	expression tag	UNP Q2PFV4
O	158	ASN	-	expression tag	UNP Q2PFV4
R	151	GLY	-	expression tag	UNP Q2PFV4
R	152	GLY	-	expression tag	UNP Q2PFV4
R	153	SER	-	expression tag	UNP Q2PFV4
R	154	GLY	-	expression tag	UNP Q2PFV4
R	155	GLY	-	expression tag	UNP Q2PFV4
R	156	GLY	-	expression tag	UNP Q2PFV4
R	157	LEU	-	expression tag	UNP Q2PFV4
R	158	ASN	-	expression tag	UNP Q2PFV4



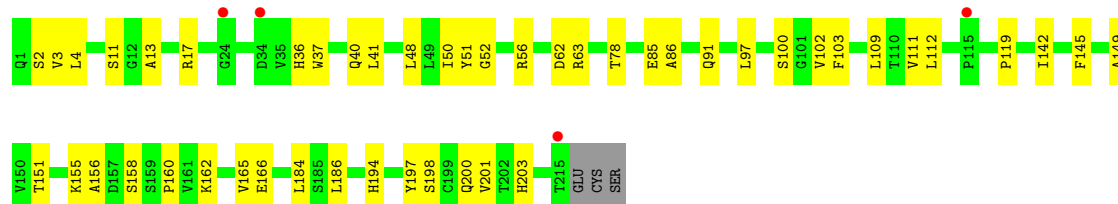
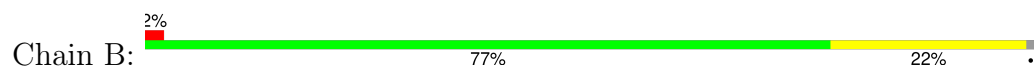
• Molecule 1: TFPI-23-Fab Heavy chain



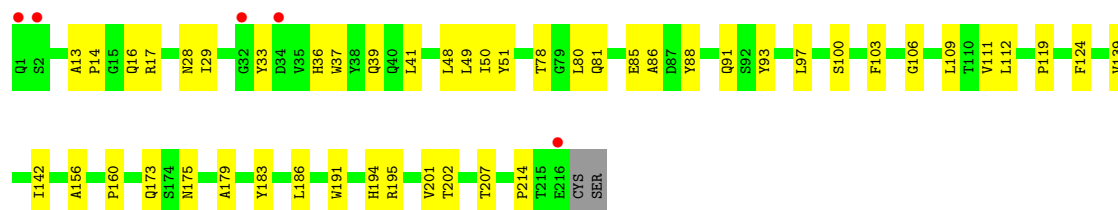
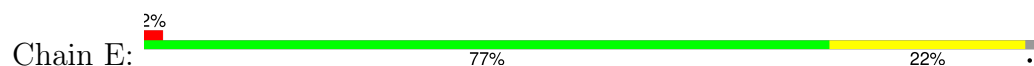
• Molecule 1: TFPI-23-Fab Heavy chain



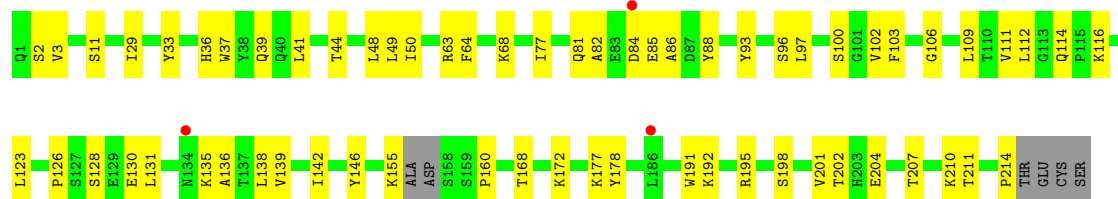
• Molecule 2: TFPI-23-Fab Light chain



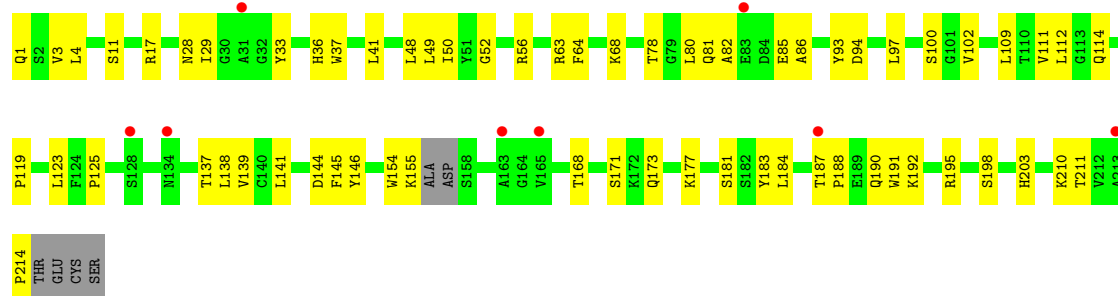
• Molecule 2: TFPI-23-Fab Light chain



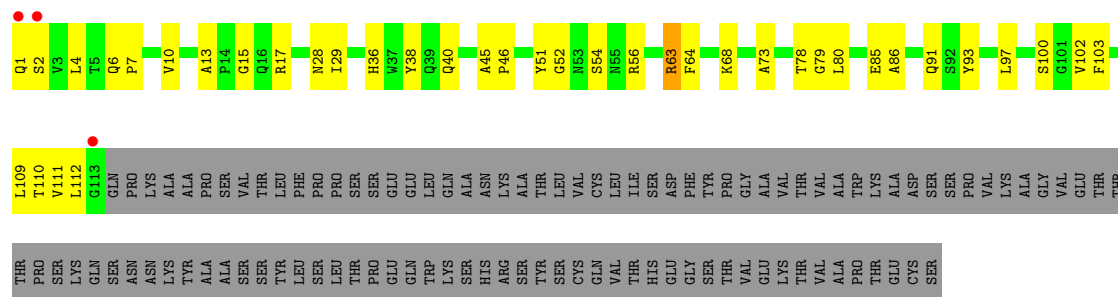
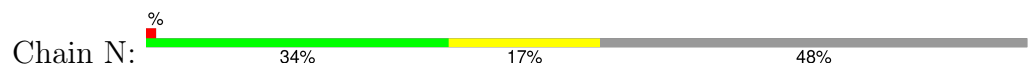
- Molecule 2: TFPI-23-Fab Light chain



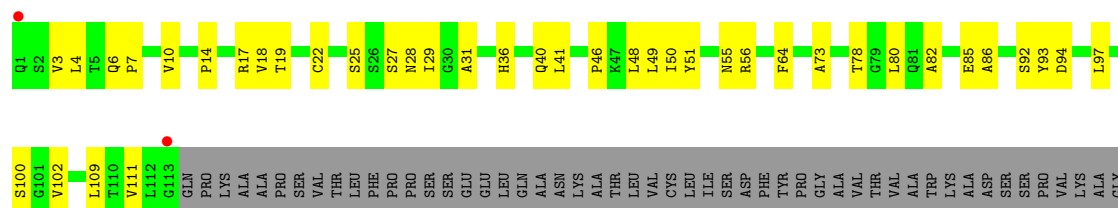
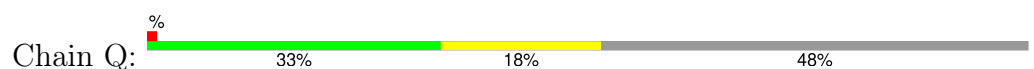
- Molecule 2: TFPI-23-Fab Light chain

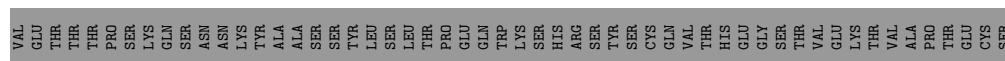


- Molecule 2: TFPI-23-Fab Light chain



- Molecule 2: TFPI-23-Fab Light chain





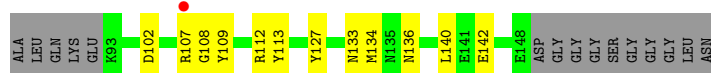
- Molecule 3: Tissue factor pathway inhibitor

Chain C: 66% 13% 21%



- Molecule 3: Tissue factor pathway inhibitor

Chain F: 62% 17% 21%



- Molecule 3: Tissue factor pathway inhibitor

Chain I: 7% 58% 21% 21%



- Molecule 3: Tissue factor pathway inhibitor

Chain L: 68% 11% 21%



- Molecule 3: Tissue factor pathway inhibitor

Chain O: 54% 25% 21%



- Molecule 3: Tissue factor pathway inhibitor

Chain R: 58% 21% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.67Å 101.37Å 119.28Å 101.83° 92.27° 96.78°	Depositor
Resolution (Å)	44.20 – 3.11 44.20 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.20-3.11) 98.4 (44.20-3.11)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.12Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.226 , 0.273 0.223 , 0.269	Depositor DCC
R_{free} test set	3050 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18693	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.17	0/1601	0.45	0/2181
1	D	0.19	0/1595	0.43	0/2173
1	G	0.17	0/1595	0.47	0/2173
1	J	0.19	0/1595	0.47	0/2173
1	M	0.20	0/904	0.43	0/1224
1	P	0.16	0/904	0.40	0/1224
2	B	0.21	0/1616	0.51	2/2207 (0.1%)
2	E	0.18	0/1625	0.45	0/2219
2	H	0.18	0/1595	0.46	0/2176
2	K	0.20	0/1595	0.51	0/2176
2	N	0.17	0/827	0.41	0/1125
2	Q	0.16	0/827	0.38	0/1125
3	C	0.20	0/472	0.44	0/631
3	F	0.19	0/472	0.48	0/631
3	I	0.25	0/472	0.57	0/631
3	L	0.16	0/472	0.48	0/631
3	O	0.18	0/472	0.49	0/631
3	R	0.19	0/472	0.45	0/631
All	All	0.19	0/19111	0.46	2/25962 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	SER	CA-C-N	6.13	131.39	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	SER	C-N-CA	6.13	131.39	121.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	63	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1566	0	1540	29	0
1	D	1560	0	1535	22	0
1	G	1560	0	1535	43	0
1	J	1560	0	1535	41	0
1	M	887	0	861	37	0
1	P	887	0	861	26	0
2	B	1578	0	1527	35	0
2	E	1587	0	1533	33	0
2	H	1558	0	1510	48	0
2	K	1558	0	1510	53	0
2	N	810	0	775	32	0
2	Q	810	0	775	32	0
3	C	462	0	416	9	0
3	F	462	0	416	10	0
3	I	462	0	416	17	0
3	L	462	0	416	9	0
3	O	462	0	416	13	0
3	R	462	0	416	14	0
All	All	18693	0	17993	444	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (444) 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:M:104:LEU:HD23	3:O:108:GLY:HA2	1.51	0.92
1:G:126:PRO:HB3	1:G:152:TYR:HB3	1.55	0.87
2:E:173:GLN:HE21	2:E:179:ALA:HB2	1.40	0.86
1:D:104:LEU:HD23	3:F:108:GLY:HA2	1.60	0.83
2:H:135:LYS:HD3	2:H:136:ALA:H	1.44	0.83
2:B:85:GLU:HB3	2:B:111:VAL:HG23	1.60	0.83
1:D:48:VAL:HG13	1:D:64:VAL:HG11	1.61	0.82
2:H:11:SER:HB2	2:H:112:LEU:HD11	1.64	0.80
2:H:97:LEU:HB3	2:H:100:SER:HB2	1.64	0.79
1:G:64:VAL:HG13	1:G:68:PHE:HB2	1.62	0.79
3:I:99:LEU:HD11	3:I:135:ASN:HB2	1.65	0.78
1:M:4:LEU:HD11	1:M:98:ILE:HG13	1.64	0.78
2:H:123:LEU:H	2:H:210:LYS:HE2	1.49	0.77
3:O:139:THR:HG23	3:O:142:GLU:H	1.51	0.76
2:H:63:ARG:HH12	2:H:81:GLN:HG3	1.50	0.75
2:B:48:LEU:HD21	2:B:51:TYR:HB3	1.68	0.75
2:K:41:LEU:HD23	2:K:86:ALA:HB2	1.68	0.75
1:G:145:LEU:HD13	1:G:218:VAL:HG11	1.69	0.74
1:G:166:LEU:HD11	1:G:189:VAL:HG21	1.70	0.74
1:M:104:LEU:HD23	3:O:108:GLY:CA	2.17	0.74
1:G:146:GLY:HA3	1:G:188:VAL:HG12	1.68	0.73
2:N:38:TYR:HE2	2:N:91:GLN:HG2	1.53	0.73
1:D:159:VAL:HG22	1:D:205:VAL:HG22	1.72	0.72
2:K:97:LEU:HB3	2:K:100:SER:HB2	1.72	0.72
1:D:104:LEU:HG	3:F:107:ARG:HB2	1.71	0.71
2:H:135:LYS:HD3	2:H:136:ALA:N	2.05	0.71
1:D:4:LEU:HD11	1:D:98:ILE:HG13	1.73	0.71
1:G:176:VAL:HB	2:H:168:THR:HG22	1.73	0.71
1:A:126:PRO:HB3	1:A:152:TYR:HB3	1.73	0.70
2:B:41:LEU:HD23	2:B:86:ALA:HB2	1.73	0.70
3:I:111:THR:HG21	3:I:124:ARG:HH21	1.57	0.69
1:M:39:GLN:HB2	1:M:45:LEU:HD23	1.74	0.69
3:C:110:ILE:HD11	2:Q:27:SER:HB2	1.75	0.69
1:J:160:SER:HB3	1:J:204:ASN:HB2	1.73	0.69
2:Q:85:GLU:HG3	2:Q:111:VAL:HG23	1.74	0.68
2:B:37:TRP:HB2	2:B:50:ILE:HB	1.76	0.67
1:J:12:VAL:HG23	1:J:118:VAL:HG12	1.75	0.67
2:N:36:HIS:HD2	2:N:52:GLY:H	1.43	0.67
2:B:11:SER:HB2	2:B:112:LEU:HD11	1.76	0.67
1:J:105:SER:HG	2:K:93:TYR:HE2	1.42	0.66
2:K:154:TRP:CD2	2:K:184:LEU:HD13	2.30	0.66
1:M:1:GLN:HG3	1:M:2:VAL:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:HG22	2:B:184:LEU:HD13	1.77	0.66
3:I:96:PHE:HZ	3:I:146:THR:HG22	1.61	0.66
2:K:155:LYS:HB3	2:K:198:SER:HB2	1.78	0.66
2:N:1:GLN:HG3	2:N:2:SER:H	1.62	0.65
1:M:105:SER:HB2	2:N:36:HIS:HE1	1.60	0.65
1:M:105:SER:HB2	2:N:36:HIS:CE1	2.32	0.65
2:K:85:GLU:HB3	2:K:111:VAL:HG23	1.78	0.65
2:Q:97:LEU:HB3	2:Q:100:SER:HB3	1.78	0.65
1:A:193:SER:HA	1:A:196:LEU:HD13	1.80	0.64
1:M:104:LEU:HG	3:O:107:ARG:HG3	1.79	0.64
1:A:67:ARG:HB3	1:A:84:ASN:O	1.97	0.63
2:N:63:ARG:NH2	2:N:80:LEU:HA	2.13	0.63
2:E:14:PRO:HD3	2:E:112:LEU:O	1.98	0.63
1:A:128:VAL:HG21	1:A:205:VAL:HG11	1.80	0.63
1:M:6:GLU:HB3	1:M:114:THR:HG22	1.80	0.63
2:H:126:PRO:HD3	2:H:138:LEU:HG	1.80	0.63
2:N:17:ARG:HG3	2:N:78:THR:HG22	1.79	0.62
1:J:87:ARG:O	1:J:118:VAL:HG21	1.99	0.62
2:E:37:TRP:HB2	2:E:50:ILE:HB	1.81	0.62
1:A:98:ILE:HD12	1:A:109:ILE:HD13	1.81	0.62
2:B:97:LEU:HB3	2:B:100:SER:HB2	1.82	0.62
1:D:126:PRO:HB3	1:D:152:TYR:HB3	1.82	0.61
2:K:144:ASP:H	2:K:173:GLN:HE22	1.46	0.61
2:N:36:HIS:CD2	2:N:52:GLY:H	2.18	0.61
2:E:156:ALA:HB1	2:E:194:HIS:CE1	2.36	0.61
1:P:104:LEU:HD22	3:R:108:GLY:CA	2.31	0.61
1:J:48:VAL:HG13	1:J:64:VAL:HG11	1.84	0.60
3:F:102:ASP:HB3	3:F:133:ASN:HD22	1.65	0.60
2:N:10:VAL:HG23	2:N:109:LEU:HD13	1.84	0.60
2:H:41:LEU:HD23	2:H:86:ALA:HB2	1.84	0.60
2:K:125:PRO:HA	2:K:138:LEU:HD23	1.82	0.60
2:H:64:PHE:HZ	2:H:84:ASP:OD1	1.85	0.60
2:B:155:LYS:HG2	2:B:198:SER:HB3	1.84	0.60
1:G:132:ALA:HB1	1:G:220:PRO:HA	1.84	0.60
2:Q:17:ARG:HG3	2:Q:78:THR:HG22	1.83	0.59
1:J:143:ALA:HB2	1:J:196:LEU:HD22	1.85	0.59
1:P:103:SER:HB3	2:Q:51:TYR:CD2	2.37	0.59
1:A:104:LEU:HD22	3:C:108:GLY:CA	2.32	0.59
1:M:106:ALA:HB2	2:N:36:HIS:CG	2.38	0.59
2:H:85:GLU:HB3	2:H:111:VAL:HG23	1.85	0.58
2:K:191:TRP:O	2:K:195:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:188:PRO:O	2:K:192:LYS:HG2	2.03	0.58
2:H:63:ARG:NH1	2:H:81:GLN:HG3	2.19	0.58
1:P:104:LEU:HD12	1:P:105:SER:N	2.19	0.57
1:A:104:LEU:HD22	3:C:108:GLY:HA3	1.84	0.57
2:Q:40:GLN:HB2	2:Q:46:PRO:HB3	1.87	0.57
1:G:153:PHE:HB2	1:G:182:LEU:HD23	1.86	0.57
2:H:37:TRP:HB2	2:H:50:ILE:HB	1.86	0.57
3:L:112:ARG:HH11	3:L:136:ASN:HD21	1.53	0.57
2:K:85:GLU:HB2	2:K:109:LEU:O	2.05	0.57
1:D:146:GLY:HA3	1:D:188:VAL:HG12	1.87	0.56
1:G:207:HIS:CD2	1:G:209:PRO:HD2	2.40	0.56
2:B:17:ARG:HG3	2:B:78:THR:HG22	1.87	0.56
2:E:85:GLU:HB2	2:E:111:VAL:HG23	1.86	0.56
1:P:104:LEU:HD22	3:R:108:GLY:HA3	1.86	0.56
2:H:142:ILE:HG12	2:H:201:VAL:HG21	1.86	0.56
1:D:106:ALA:HB2	2:E:36:HIS:CG	2.40	0.56
2:E:156:ALA:HB1	2:E:194:HIS:ND1	2.21	0.56
1:A:103:SER:HB3	2:B:51:TYR:CD2	2.41	0.56
2:B:2:SER:HB2	2:B:103:PHE:O	2.06	0.56
1:J:153:PHE:HB2	1:J:182:LEU:HD23	1.88	0.56
3:R:113:TYR:CE2	3:R:140:LEU:HB2	2.41	0.56
2:H:123:LEU:HD12	2:H:139:VAL:O	2.06	0.55
2:H:64:PHE:CZ	2:H:84:ASP:OD1	2.60	0.55
2:K:195:ARG:HB3	2:K:214:PRO:HG3	1.88	0.55
1:P:4:LEU:HD21	1:P:34:MET:HE1	1.89	0.55
3:O:102:ASP:HB3	3:O:133:ASN:HD22	1.71	0.55
1:J:175:ALA:HB2	1:J:185:LEU:HD23	1.88	0.55
1:G:130:PRO:HD3	1:G:216:LYS:HG2	1.88	0.55
2:B:186:LEU:HD21	2:B:197:TYR:CZ	2.42	0.55
3:I:99:LEU:CD1	3:I:135:ASN:HB2	2.34	0.55
1:M:112:GLN:HA	2:N:45:ALA:HB2	1.87	0.55
2:E:80:LEU:HD21	2:E:109:LEU:HD21	1.89	0.55
1:D:100:GLY:HA2	1:D:103:SER:O	2.07	0.54
2:E:41:LEU:HD13	2:E:86:ALA:HB2	1.89	0.54
2:K:114:GLN:HB2	2:K:146:TYR:CZ	2.42	0.54
1:M:30:SER:HB3	1:M:74:ASN:HB3	1.88	0.54
1:J:178:GLN:HG2	1:J:182:LEU:O	2.07	0.54
2:K:119:PRO:HB3	2:K:145:PHE:HB3	1.90	0.54
2:N:97:LEU:HB3	2:N:100:SER:HB3	1.89	0.54
2:B:85:GLU:HA	2:B:109:LEU:HD22	1.90	0.54
1:D:126:PRO:HD2	1:D:212:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:13:ALA:HA	2:N:112:LEU:HB2	1.89	0.54
2:K:82:ALA:O	2:K:85:GLU:HG2	2.08	0.54
1:G:34:MET:HB3	1:G:79:LEU:HD22	1.89	0.54
1:G:104:LEU:HD13	3:I:108:GLY:HA3	1.90	0.54
1:J:105:SER:OG	2:K:93:TYR:HE2	1.89	0.54
2:K:144:ASP:H	2:K:173:GLN:NE2	2.06	0.54
2:K:139:VAL:HG23	2:K:183:TYR:CD1	2.43	0.54
1:M:100:GLY:HA2	1:M:103:SER:O	2.08	0.53
2:Q:56:ARG:HD3	2:Q:64:PHE:O	2.09	0.53
2:B:40:GLN:O	2:B:86:ALA:HB1	2.09	0.53
1:P:12:VAL:HG11	1:P:86:LEU:HD13	1.90	0.53
1:A:12:VAL:HG21	1:A:86:LEU:HD13	1.90	0.53
2:N:85:GLU:HG3	2:N:110:THR:HA	1.89	0.53
2:Q:82:ALA:HA	2:Q:111:VAL:HG21	1.91	0.53
2:K:145:PHE:HB2	2:K:203:HIS:CD2	2.44	0.53
1:G:5:VAL:HG13	1:G:112:GLN:HE22	1.73	0.53
1:J:5:VAL:HG13	1:J:112:GLN:NE2	2.24	0.53
1:J:126:PRO:HB3	1:J:152:TYR:HB3	1.91	0.53
2:K:81:GLN:O	2:K:111:VAL:HG21	2.09	0.53
1:M:12:VAL:HG13	1:M:118:VAL:HG22	1.90	0.53
1:A:103:SER:OG	1:A:106:ALA:HB3	2.08	0.53
3:F:113:TYR:CE2	3:F:140:LEU:HB2	2.44	0.53
2:B:142:ILE:HG12	2:B:201:VAL:HG21	1.91	0.52
1:G:159:VAL:HG22	1:G:205:VAL:HG22	1.91	0.52
1:D:67:ARG:HB3	1:D:84:ASN:O	2.09	0.52
2:E:97:LEU:HB3	2:E:100:SER:HB2	1.91	0.52
2:Q:31:ALA:HA	3:R:138:GLU:OE2	2.09	0.52
2:B:4:LEU:HG	2:B:102:VAL:HG12	1.91	0.52
2:H:146:TYR:HB2	2:H:177:LYS:HD3	1.90	0.52
3:L:112:ARG:HD3	3:L:136:ASN:HD21	1.74	0.52
2:B:156:ALA:HB1	2:B:194:HIS:ND1	2.25	0.52
2:H:81:GLN:O	2:H:111:VAL:HG21	2.10	0.52
2:B:13:ALA:HA	2:B:112:LEU:HB2	1.91	0.52
1:G:91:THR:HG23	1:G:116:VAL:O	2.10	0.52
2:K:94:ASP:HB2	2:K:102:VAL:HG21	1.92	0.52
2:H:96:SER:HA	3:I:134:MET:HE3	1.92	0.52
2:B:119:PRO:HG3	2:B:203:HIS:HB2	1.92	0.51
2:E:39:GLN:HB2	2:E:49:LEU:HD12	1.91	0.51
2:K:17:ARG:HG3	2:K:78:THR:HG22	1.92	0.51
2:H:82:ALA:O	2:H:85:GLU:HG2	2.10	0.51
3:R:98:PHE:HA	3:R:117:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:LYS:HA	2:H:160:PRO:HA	1.92	0.51
1:J:208:LYS:HB2	1:J:209:PRO:HD3	1.92	0.51
3:F:134:MET:HE3	3:R:109:TYR:HD2	1.75	0.51
2:H:85:GLU:HB2	2:H:109:LEU:O	2.10	0.51
1:A:148:LEU:HD22	1:A:150:LYS:HB2	1.93	0.51
1:J:152:TYR:CZ	1:J:183:TYR:HB2	2.45	0.51
2:Q:28:ASN:OD1	2:Q:29:ILE:HG12	2.10	0.51
2:Q:25:SER:HB3	2:Q:28:ASN:ND2	2.26	0.51
1:A:1:GLN:HG2	1:A:2:VAL:H	1.76	0.50
2:Q:6:GLN:HG2	2:Q:7:PRO:HD2	1.93	0.50
1:G:104:LEU:HD13	3:I:108:GLY:CA	2.41	0.50
3:L:112:ARG:HH21	3:L:138:GLU:HB2	1.76	0.50
3:C:113:TYR:CE2	3:C:140:LEU:HB2	2.46	0.50
2:B:63:ARG:HD2	2:B:78:THR:O	2.12	0.50
1:J:88:ALA:HA	1:J:118:VAL:HG23	1.93	0.50
1:P:6:GLU:OE2	1:P:111:GLY:HA3	2.12	0.50
1:A:104:LEU:HB2	3:C:107:ARG:H	1.77	0.50
2:H:33:TYR:CD1	2:H:93:TYR:HB2	2.47	0.50
3:I:113:TYR:CE1	3:I:124:ARG:HG2	2.47	0.50
1:M:103:SER:OG	1:M:106:ALA:HB3	2.11	0.50
2:Q:10:VAL:O	2:Q:109:LEU:HA	2.11	0.50
2:K:49:LEU:HD11	2:K:64:PHE:CD2	2.46	0.50
2:B:194:HIS:HB2	2:B:197:TYR:CE2	2.47	0.50
2:K:191:TRP:CD1	2:K:195:ARG:HE	2.30	0.50
1:G:64:VAL:CG1	1:G:68:PHE:HB2	2.38	0.49
1:M:22:CYS:O	1:M:78:THR:HA	2.12	0.49
1:D:153:PHE:HB2	1:D:182:LEU:HD23	1.92	0.49
2:E:160:PRO:HG3	3:O:117:ASN:HD21	1.77	0.49
1:J:143:ALA:HB1	1:J:196:LEU:HD13	1.95	0.49
1:M:5:VAL:O	1:M:22:CYS:HA	2.12	0.49
1:A:108:ASP:HB2	1:A:109:ILE:HD12	1.94	0.49
3:F:112:ARG:HD2	3:F:136:ASN:OD1	2.12	0.49
3:I:98:PHE:HA	3:I:117:ASN:OD1	2.13	0.49
1:A:5:VAL:HG23	1:A:23:ALA:HB3	1.93	0.49
2:E:85:GLU:HG3	2:E:109:LEU:O	2.13	0.49
2:N:38:TYR:CE2	2:N:91:GLN:HG2	2.42	0.49
2:Q:3:VAL:HB	2:Q:102:VAL:CG1	2.43	0.49
1:A:175:ALA:HB2	1:A:185:LEU:HD23	1.95	0.49
1:P:22:CYS:O	1:P:78:THR:HA	2.13	0.49
1:D:103:SER:OG	1:D:106:ALA:HB3	2.13	0.49
1:J:100:GLY:HA2	1:J:103:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:123:LEU:H	2:K:210:LYS:HD3	1.78	0.49
1:M:82:GLN:HG3	1:M:84:ASN:HD21	1.78	0.49
3:I:94:PRO:HB2	3:I:98:PHE:CE2	2.48	0.48
2:H:49:LEU:HD21	2:H:64:PHE:CD2	2.48	0.48
1:J:176:VAL:HB	2:K:168:THR:OG1	2.13	0.48
1:M:73:ASP:CG	1:M:76:LYS:HG2	2.38	0.48
2:E:49:LEU:HD22	2:E:50:ILE:HG12	1.95	0.48
2:N:4:LEU:HG	2:N:102:VAL:HG12	1.96	0.48
1:G:126:PRO:HB2	1:G:149:VAL:HG13	1.95	0.48
2:H:202:THR:HG22	2:H:207:THR:HG23	1.95	0.48
1:J:206:ASN:HD22	1:J:213:LYS:HB2	1.79	0.48
3:I:134:MET:C	3:I:136:ASN:H	2.22	0.48
1:J:173:PHE:HB3	2:K:181:SER:HB3	1.95	0.48
2:K:4:LEU:HG	2:K:102:VAL:HG12	1.94	0.48
1:G:60:TYR:CZ	1:G:70:ILE:HG22	2.49	0.48
1:J:150:LYS:HG2	1:J:151:ASP:OD2	2.14	0.48
2:Q:80:LEU:HD21	2:Q:109:LEU:HD21	1.96	0.48
1:D:34:MET:HB3	1:D:79:LEU:HD22	1.96	0.47
1:G:100:GLY:HA2	1:G:103:SER:O	2.13	0.47
3:O:144:LYS:HE3	3:O:148:GLU:OE1	2.14	0.47
2:Q:48:LEU:HD21	2:Q:51:TYR:HB3	1.96	0.47
2:B:85:GLU:HB2	2:B:109:LEU:O	2.13	0.47
2:B:155:LYS:HA	2:B:160:PRO:HA	1.96	0.47
1:J:173:PHE:CZ	2:K:141:LEU:HB3	2.49	0.47
1:P:106:ALA:HB2	2:Q:36:HIS:CG	2.50	0.47
1:A:146:GLY:HA3	1:A:188:VAL:HG12	1.95	0.47
1:J:12:VAL:O	1:J:118:VAL:HA	2.14	0.47
2:N:15:GLY:HA2	2:N:79:GLY:HA2	1.95	0.47
2:Q:18:VAL:HG21	2:Q:109:LEU:HD11	1.95	0.47
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.96	0.47
1:G:91:THR:OG1	1:G:118:VAL:HG22	2.15	0.47
1:G:128:VAL:HG22	1:G:149:VAL:HG22	1.96	0.47
1:G:172:THR:HG23	1:G:187:SER:HB2	1.97	0.47
3:R:140:LEU:HD21	3:R:144:LYS:HE2	1.97	0.47
1:M:5:VAL:HB	1:M:23:ALA:HB3	1.96	0.47
1:P:18:LEU:HD23	1:P:19:ARG:N	2.29	0.47
3:I:99:LEU:O	3:I:99:LEU:HD12	2.14	0.47
1:D:83:MET:HE3	1:D:86:LEU:HD21	1.97	0.47
2:E:17:ARG:HG3	2:E:78:THR:HG22	1.96	0.47
2:K:28:ASN:OD1	2:K:29:ILE:HG12	2.14	0.47
2:Q:41:LEU:HD23	2:Q:86:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD23	1:A:96:CYS:SG	2.55	0.46
1:J:5:VAL:HG13	1:J:112:GLN:HE22	1.78	0.46
3:C:109:TYR:CD2	3:R:96:PHE:HE2	2.33	0.46
1:G:105:SER:HB2	2:H:93:TYR:HE2	1.81	0.46
1:G:145:LEU:HD13	1:G:218:VAL:CG1	2.43	0.46
2:K:146:TYR:O	2:K:203:HIS:HE1	1.97	0.46
1:J:33:ALA:HB1	3:L:105:ILE:HD12	1.98	0.46
1:J:126:PRO:HB2	1:J:149:VAL:HG13	1.98	0.46
1:A:106:ALA:HB2	2:B:36:HIS:CG	2.51	0.46
2:Q:22:CYS:HB3	2:Q:73:ALA:O	2.16	0.46
2:E:28:ASN:OD1	2:E:29:ILE:HG12	2.15	0.46
1:P:34:MET:HB3	1:P:79:LEU:HD22	1.97	0.46
2:B:162:LYS:HD3	2:B:162:LYS:HA	1.72	0.46
1:D:104:LEU:HD23	3:F:108:GLY:CA	2.38	0.46
1:D:196:LEU:HD22	1:D:220:PRO:HG3	1.96	0.46
2:K:36:HIS:CE1	2:K:52:GLY:H	2.33	0.46
2:K:137:THR:HG23	2:K:184:LEU:O	2.15	0.46
1:M:99:LEU:HB2	1:M:107:PHE:HD1	1.80	0.46
1:P:52:SER:HB2	1:P:57:SER:HB2	1.97	0.46
3:R:112:ARG:HD3	3:R:138:GLU:HA	1.98	0.46
2:K:144:ASP:HA	2:K:177:LYS:HB2	1.98	0.46
1:M:34:MET:HB3	1:M:79:LEU:HD22	1.98	0.46
1:P:91:THR:HG23	1:P:116:VAL:O	2.16	0.46
1:D:106:ALA:HB2	2:E:36:HIS:ND1	2.31	0.46
2:H:116:LYS:HD3	2:H:204:GLU:HG3	1.98	0.46
2:E:173:GLN:HB2	2:E:175:ASN:OD1	2.15	0.45
1:G:12:VAL:O	1:G:118:VAL:HA	2.15	0.45
2:B:145:PHE:HB2	2:B:203:HIS:CE1	2.52	0.45
2:E:81:GLN:O	2:E:111:VAL:HG21	2.17	0.45
3:F:109:TYR:HA	3:F:127:TYR:O	2.17	0.45
2:H:88:TYR:O	2:H:106:GLY:HA2	2.17	0.45
2:E:202:THR:HG23	2:E:207:THR:HG22	1.98	0.45
1:J:108:ASP:HA	2:K:48:LEU:HD22	1.98	0.45
3:L:112:ARG:NH1	3:L:136:ASN:HD21	2.14	0.45
1:P:104:LEU:HB2	3:R:107:ARG:H	1.82	0.45
1:A:20:LEU:HD12	1:A:81:LEU:HD23	1.99	0.45
2:B:151:THR:O	2:B:201:VAL:HA	2.17	0.45
2:K:3:VAL:HB	2:K:102:VAL:HG11	1.98	0.45
1:A:98:ILE:O	1:A:107:PHE:HA	2.17	0.45
2:K:80:LEU:HD21	2:K:109:LEU:HD21	1.98	0.45
1:P:6:GLU:OE2	1:P:96:CYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:41:LEU:O	2:H:44:THR:HG22	2.16	0.45
2:K:154:TRP:CG	2:K:184:LEU:HD13	2.52	0.45
2:E:88:TYR:O	2:E:106:GLY:HA2	2.16	0.45
1:M:106:ALA:HB2	2:N:36:HIS:CD2	2.52	0.45
2:H:198:SER:OG	2:H:211:THR:HG22	2.17	0.44
1:M:61:ALA:O	1:M:64:VAL:HG22	2.17	0.44
2:B:36:HIS:HD1	2:B:52:GLY:H	1.65	0.44
1:G:108:ASP:HA	2:H:48:LEU:HD22	2.00	0.44
2:H:114:GLN:CB	2:H:177:LYS:HZ1	2.30	0.44
1:G:126:PRO:HD3	1:G:207:HIS:ND1	2.33	0.44
2:H:155:LYS:HB2	2:H:198:SER:HB2	2.00	0.44
2:K:37:TRP:HB2	2:K:50:ILE:HB	1.99	0.44
3:L:112:ARG:HD3	3:L:136:ASN:ND2	2.32	0.44
1:M:19:ARG:HB2	1:M:82:GLN:NE2	2.33	0.44
1:P:100:GLY:HA2	1:P:103:SER:O	2.17	0.44
2:Q:25:SER:HB3	2:Q:28:ASN:HD21	1.83	0.44
1:D:22:CYS:O	1:D:78:THR:HA	2.18	0.44
1:M:60:TYR:HB3	1:M:64:VAL:CG2	2.48	0.44
2:N:93:TYR:CE2	3:O:130:CYS:HB2	2.53	0.44
1:A:104:LEU:HD12	1:A:105:SER:N	2.32	0.44
3:C:141:GLU:OE2	3:L:123:GLU:HG2	2.18	0.44
2:E:13:ALA:HB3	2:E:16:GLN:HG2	2.00	0.44
3:C:134:MET:O	3:C:134:MET:HG3	2.16	0.44
2:E:195:ARG:O	2:E:214:PRO:HD2	2.18	0.44
1:G:19:ARG:HB2	1:G:82:GLN:OE1	2.17	0.44
1:G:169:GLY:C	1:G:189:VAL:HG23	2.42	0.44
2:H:191:TRP:CE3	2:H:192:LYS:HG3	2.53	0.44
1:J:166:LEU:HD21	1:J:189:VAL:HG21	2.00	0.44
2:B:56:ARG:CZ	2:B:62:ASP:HA	2.47	0.44
1:G:104:LEU:H	1:G:104:LEU:HG	1.64	0.43
1:G:106:ALA:HB2	2:H:36:HIS:ND1	2.33	0.43
2:K:49:LEU:HD13	2:K:50:ILE:HG12	1.99	0.43
1:M:60:TYR:HB3	1:M:64:VAL:HG21	1.99	0.43
2:E:139:VAL:HG22	2:E:183:TYR:CD1	2.52	0.43
1:G:11:LEU:HA	1:G:117:THR:O	2.18	0.43
1:J:127:SER:OG	1:J:150:LYS:HB2	2.17	0.43
2:K:3:VAL:HB	2:K:102:VAL:CG1	2.48	0.43
3:O:109:TYR:HA	3:O:127:TYR:O	2.18	0.43
1:A:148:LEU:CD2	1:A:150:LYS:HB2	2.49	0.43
1:J:91:THR:OG1	1:J:118:VAL:HG22	2.18	0.43
1:P:65:LYS:HZ3	1:P:65:LYS:HG2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:98:ILE:HD12	1:P:109:ILE:HB	2.00	0.43
1:G:106:ALA:HB2	2:H:36:HIS:CG	2.53	0.43
1:A:99:LEU:HD12	1:A:107:PHE:CE1	2.54	0.43
1:G:48:VAL:HG13	1:G:64:VAL:HG21	1.99	0.43
2:H:29:ILE:CG2	2:H:68:LYS:HE3	2.49	0.43
2:H:131:LEU:HD22	2:H:192:LYS:HE2	2.01	0.43
1:M:19:ARG:HB2	1:M:82:GLN:HE22	1.84	0.43
2:Q:14:PRO:HA	2:Q:80:LEU:O	2.18	0.43
2:Q:94:ASP:HB2	2:Q:102:VAL:HG21	1.99	0.43
2:B:11:SER:HB2	2:B:112:LEU:CD1	2.47	0.43
2:E:142:ILE:HG12	2:E:201:VAL:HG21	1.99	0.43
2:H:172:LYS:HG2	2:H:178:TYR:CE2	2.54	0.43
3:L:109:TYR:HA	3:L:127:TYR:O	2.19	0.43
1:M:73:ASP:OD1	1:M:76:LYS:HG2	2.19	0.43
1:G:207:HIS:HD2	1:G:209:PRO:HD2	1.83	0.43
2:H:195:ARG:HD3	2:H:214:PRO:HG2	2.00	0.43
3:I:113:TYR:CE1	3:I:140:LEU:HG	2.54	0.43
2:Q:3:VAL:HB	2:Q:102:VAL:HG13	2.01	0.43
2:B:149:ALA:O	2:B:203:HIS:HD2	2.02	0.43
3:I:99:LEU:HD12	3:I:99:LEU:C	2.44	0.43
1:J:106:ALA:HB2	2:K:36:HIS:CG	2.54	0.43
2:K:139:VAL:HG23	2:K:183:TYR:CE1	2.53	0.43
1:P:33:ALA:HA	1:P:72:ARG:HH12	1.83	0.43
1:P:34:MET:SD	1:P:98:ILE:HA	2.58	0.43
2:K:11:SER:HB3	2:K:112:LEU:HD21	2.01	0.43
2:K:63:ARG:HB3	2:K:78:THR:O	2.19	0.43
2:N:6:GLN:HG2	2:N:7:PRO:HD2	2.01	0.43
2:K:198:SER:HA	2:K:211:THR:HA	2.01	0.42
1:D:131:LEU:HB3	2:E:124:PHE:CD1	2.54	0.42
1:G:103:SER:OG	1:G:106:ALA:HB3	2.19	0.42
3:I:96:PHE:HZ	3:I:146:THR:CG2	2.29	0.42
1:P:40:ALA:HA	1:P:92:ALA:HA	2.00	0.42
2:Q:40:GLN:O	2:Q:86:ALA:HB1	2.18	0.42
2:E:119:PRO:HB2	2:E:142:ILE:HG23	2.00	0.42
1:A:97:ALA:HB1	1:A:107:PHE:HB3	2.00	0.42
2:E:33:TYR:CD1	2:E:93:TYR:HB2	2.54	0.42
1:G:87:ARG:O	1:G:118:VAL:HG21	2.20	0.42
1:J:219:GLU:HA	1:J:220:PRO:HD3	1.78	0.42
1:D:128:VAL:HB	1:D:214:VAL:HG11	2.02	0.42
2:E:48:LEU:HD21	2:E:51:TYR:HB3	2.01	0.42
2:E:139:VAL:HG22	2:E:183:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:LEU:HD11	2:E:191:TRP:HB2	2.02	0.42
3:F:113:TYR:CD2	3:F:140:LEU:HB2	2.55	0.42
1:G:112:GLN:HG2	1:G:113:GLY:N	2.34	0.42
1:G:129:PHE:CE2	2:H:130:GLU:HG3	2.55	0.42
2:K:119:PRO:HG3	2:K:203:HIS:HB2	2.01	0.42
1:M:4:LEU:HD22	1:M:22:CYS:SG	2.60	0.42
2:N:40:GLN:O	2:N:86:ALA:HB1	2.19	0.42
2:N:68:LYS:HA	2:N:73:ALA:HA	2.01	0.42
3:R:144:LYS:HG2	3:R:148:GLU:CD	2.44	0.42
2:H:112:LEU:HA	2:H:146:TYR:OH	2.19	0.42
3:O:111:THR:OG1	3:O:124:ARG:HD2	2.19	0.42
1:G:59:TYR:CE1	3:I:105:ILE:HD11	2.55	0.42
2:N:85:GLU:HB2	2:N:111:VAL:HG23	2.01	0.42
1:J:157:VAL:HG21	1:J:185:LEU:HD21	2.02	0.42
2:B:155:LYS:HD3	2:B:200:GLN:NE2	2.34	0.42
3:C:134:MET:C	3:C:136:ASN:H	2.27	0.42
1:G:71:SER:OG	1:G:80:TYR:HB2	2.20	0.42
2:N:40:GLN:HA	2:N:46:PRO:HA	2.01	0.42
2:N:63:ARG:H	2:N:63:ARG:HG2	1.46	0.42
2:N:80:LEU:CD1	2:N:111:VAL:HG13	2.49	0.42
1:M:91:THR:HG23	1:M:116:VAL:O	2.19	0.41
3:O:113:TYR:CE2	3:O:140:LEU:HB2	2.55	0.41
2:Q:51:TYR:CZ	2:Q:55:ASN:HB3	2.54	0.41
1:M:76:LYS:HA	1:M:76:LYS:HD3	1.80	0.41
1:P:29:PHE:HD2	1:P:74:ASN:HA	1.85	0.41
1:A:100:GLY:HA2	1:A:103:SER:O	2.19	0.41
1:A:178:GLN:HA	2:B:166:GLU:OE1	2.19	0.41
2:B:3:VAL:HB	2:B:102:VAL:HG11	2.02	0.41
1:D:157:VAL:HB	1:D:185:LEU:HD21	2.03	0.41
1:M:68:PHE:HA	1:M:82:GLN:O	2.20	0.41
2:N:2:SER:HA	2:N:103:PHE:O	2.20	0.41
3:F:142:GLU:OE2	3:R:126:LYS:HE2	2.20	0.41
1:J:100:GLY:O	3:L:107:ARG:HD3	2.19	0.41
2:K:33:TYR:CD1	2:K:93:TYR:HB2	2.55	0.41
1:P:105:SER:OG	2:Q:36:HIS:CE1	2.73	0.41
1:P:105:SER:HB2	2:Q:93:TYR:HE2	1.86	0.41
3:R:134:MET:O	3:R:134:MET:HG3	2.19	0.41
1:J:174:PRO:HG2	2:K:171:SER:OG	2.20	0.41
2:N:63:ARG:HH22	2:N:80:LEU:HA	1.84	0.41
1:M:103:SER:HB3	2:N:51:TYR:CD2	2.55	0.41
2:N:28:ASN:OD1	2:N:29:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:56:ARG:HD3	2:N:64:PHE:O	2.20	0.41
1:P:64:VAL:O	1:P:65:LYS:HG2	2.20	0.41
2:E:160:PRO:HG3	3:O:117:ASN:ND2	2.35	0.41
1:G:104:LEU:HB3	3:I:108:GLY:H	1.85	0.41
2:H:172:LYS:HE2	2:H:172:LYS:HB3	1.76	0.41
2:Q:49:LEU:HD13	2:Q:50:ILE:HG13	2.03	0.41
1:J:177:LEU:HD13	1:J:183:TYR:CE1	2.56	0.41
1:M:22:CYS:HB3	1:M:79:LEU:HB3	2.03	0.41
1:M:68:PHE:CD1	1:M:83:MET:HA	2.56	0.41
2:Q:4:LEU:HG	2:Q:102:VAL:HG12	2.02	0.41
2:H:77:ILE:HG21	2:H:84:ASP:OD2	2.20	0.41
1:J:146:GLY:HA3	1:J:188:VAL:HG12	2.02	0.41
1:M:13:GLN:HG2	1:M:14:PRO:HD2	2.03	0.41
3:O:134:MET:C	3:O:136:ASN:H	2.29	0.41
2:H:128:SER:HA	2:H:131:LEU:HD12	2.02	0.41
1:J:34:MET:HB3	1:J:79:LEU:HD22	2.02	0.41
2:K:50:ILE:HD13	2:K:56:ARG:HG3	2.02	0.41
2:Q:19:THR:O	2:Q:19:THR:HG23	2.21	0.41
3:R:93:LYS:HD3	3:R:98:PHE:CZ	2.55	0.41
2:H:3:VAL:HB	2:H:102:VAL:HG11	2.03	0.40
2:K:1:GLN:HG3	2:N:54:SER:HB2	2.02	0.40
2:K:29:ILE:HG23	2:K:68:LYS:HD2	2.02	0.40
1:A:129:PHE:HE2	1:A:150:LYS:HE2	1.86	0.40
2:H:2:SER:HB2	2:H:103:PHE:O	2.21	0.40
2:H:39:GLN:HB2	2:H:49:LEU:HD22	2.03	0.40
1:J:97:ALA:HB1	1:J:107:PHE:HB3	2.02	0.40
1:J:132:ALA:HB1	1:J:220:PRO:HA	2.02	0.40
1:P:68:PHE:CG	1:P:83:MET:HG2	2.57	0.40
2:Q:92:SER:O	2:Q:102:VAL:HB	2.22	0.40
2:B:91:GLN:HB2	2:B:103:PHE:CE1	2.57	0.40
2:E:91:GLN:HB2	2:E:103:PHE:CE1	2.57	0.40
1:J:172:THR:HG23	1:J:187:SER:HB2	2.04	0.40
2:K:187:THR:OG1	2:K:190:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/223 (94%)	204 (98%)	5 (2%)	0	100	100
1	D	208/223 (93%)	204 (98%)	3 (1%)	1 (0%)	24	55
1	G	208/223 (93%)	203 (98%)	4 (2%)	1 (0%)	24	55
1	J	208/223 (93%)	202 (97%)	5 (2%)	1 (0%)	24	55
1	M	118/223 (53%)	117 (99%)	1 (1%)	0	100	100
1	P	118/223 (53%)	117 (99%)	1 (1%)	0	100	100
2	B	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
2	E	214/218 (98%)	209 (98%)	5 (2%)	0	100	100
2	H	208/218 (95%)	205 (99%)	3 (1%)	0	100	100
2	K	208/218 (95%)	201 (97%)	7 (3%)	0	100	100
2	N	111/218 (51%)	106 (96%)	5 (4%)	0	100	100
2	Q	111/218 (51%)	110 (99%)	1 (1%)	0	100	100
3	C	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
3	F	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
3	I	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
3	L	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
3	O	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
3	R	54/71 (76%)	51 (94%)	3 (6%)	0	100	100
All	All	2458/3072 (80%)	2394 (97%)	61 (2%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	65	LYS
1	G	151	ASP
1	J	150	LYS

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	175/183 (96%)	174 (99%)	1 (1%)	78	81
1	D	174/183 (95%)	173 (99%)	1 (1%)	78	81
1	G	174/183 (95%)	174 (100%)	0	100	100
1	J	174/183 (95%)	173 (99%)	1 (1%)	78	81
1	M	94/183 (51%)	94 (100%)	0	100	100
1	P	94/183 (51%)	94 (100%)	0	100	100
2	B	177/180 (98%)	177 (100%)	0	100	100
2	E	178/180 (99%)	178 (100%)	0	100	100
2	H	175/180 (97%)	175 (100%)	0	100	100
2	K	175/180 (97%)	175 (100%)	0	100	100
2	N	89/180 (49%)	89 (100%)	0	100	100
2	Q	89/180 (49%)	89 (100%)	0	100	100
3	C	51/59 (86%)	51 (100%)	0	100	100
3	F	51/59 (86%)	51 (100%)	0	100	100
3	I	51/59 (86%)	51 (100%)	0	100	100
3	L	51/59 (86%)	51 (100%)	0	100	100
3	O	51/59 (86%)	51 (100%)	0	100	100
3	R	51/59 (86%)	51 (100%)	0	100	100
All	All	2074/2532 (82%)	2071 (100%)	3 (0%)	88	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	CYS
1	D	96	CYS
1	J	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	74	ASN
1	A	206	ASN
2	B	200	GLN
1	D	171	HIS
1	D	178	GLN
2	E	173	GLN
2	E	176	ASN
2	E	194	HIS
3	F	117	ASN
3	I	133	ASN
2	K	81	GLN
2	K	132	GLN
2	K	176	ASN
2	K	190	GLN
3	L	136	ASN
1	M	84	ASN
2	N	36	HIS
2	N	55	ASN
3	O	117	ASN
2	Q	81	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 [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	213/223 (95%)	-0.10	3 (1%) 73 53	36, 67, 127, 149	0
1	D	212/223 (95%)	-0.22	1 (0%) 87 73	41, 57, 87, 125	0
1	G	212/223 (95%)	0.41	7 (3%) 49 29	59, 89, 165, 189	0
1	J	212/223 (95%)	0.27	7 (3%) 49 29	42, 73, 186, 238	0
1	M	120/223 (53%)	0.38	3 (2%) 58 37	60, 93, 114, 139	0
1	P	120/223 (53%)	0.28	3 (2%) 58 37	63, 106, 137, 173	0
2	B	215/218 (98%)	0.20	4 (1%) 66 45	39, 86, 130, 155	0
2	E	216/218 (99%)	-0.03	5 (2%) 61 39	43, 70, 97, 126	0
2	H	212/218 (97%)	0.16	3 (1%) 73 53	53, 86, 195, 270	0
2	K	212/218 (97%)	0.30	8 (3%) 44 25	39, 90, 202, 252	0
2	N	113/218 (51%)	0.24	3 (2%) 56 35	51, 86, 137, 163	0
2	Q	113/218 (51%)	0.27	2 (1%) 67 46	57, 77, 112, 149	0
3	C	56/71 (78%)	-0.29	0 100 100	42, 53, 72, 86	0
3	F	56/71 (78%)	-0.33	1 (1%) 67 46	41, 49, 72, 89	0
3	I	56/71 (78%)	0.67	5 (8%) 15 8	79, 140, 170, 260	0
3	L	56/71 (78%)	-0.28	0 100 100	41, 51, 70, 86	0
3	O	56/71 (78%)	-0.32	0 100 100	40, 51, 69, 93	0
3	R	56/71 (78%)	-0.25	0 100 100	44, 56, 81, 106	0
All	All	2506/3072 (81%)	0.12	55 (2%) 62 41	36, 74, 163, 270	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	111	GLY	4.5
2	E	1	GLN	4.1
1	A	104	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	149	VAL	3.3
1	P	104	LEU	3.2
1	M	1	GLN	3.2
2	H	186	LEU	3.2
1	G	157	VAL	3.2
1	J	148	LEU	3.1
1	J	150	LYS	3.1
2	N	113	GLY	2.9
1	P	66	GLY	2.9
2	B	34	ASP	2.8
2	K	31	ALA	2.8
2	K	134	ASN	2.7
1	J	184	SER	2.7
2	K	83	GLU	2.7
2	N	1	GLN	2.7
2	K	163	ALA	2.7
3	I	109	TYR	2.7
1	G	133	PRO	2.6
3	I	94	PRO	2.6
1	J	133	PRO	2.5
2	K	128	SER	2.5
2	B	215	THR	2.5
1	G	220	PRO	2.5
2	N	2	SER	2.5
1	D	104	LEU	2.5
1	A	103	SER	2.4
1	M	66	GLY	2.4
2	E	2	SER	2.4
2	H	134	ASN	2.3
2	Q	1	GLN	2.3
1	J	142	THR	2.3
2	K	165	VAL	2.3
2	E	32	GLY	2.3
3	I	96	PHE	2.3
3	F	107	ARG	2.3
1	G	104	LEU	2.3
2	K	187	THR	2.3
1	A	65	LYS	2.3
3	I	101	GLU	2.2
2	K	213	ALA	2.2
1	G	217	LYS	2.2
1	G	145	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	34	ASP	2.2
1	G	128	VAL	2.2
2	Q	113	GLY	2.1
2	B	24	GLY	2.1
1	M	37	VAL	2.1
2	B	115	PRO	2.1
3	I	93	LYS	2.0
1	J	186	SER	2.0
2	H	84	ASP	2.0
2	E	216	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.