



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:40 AM UTC

PDB ID : 6JOB / pdb_00006job
Title : Ferritin variant with "GMG" motif
Authors : Zheng, B.W.; Zhou, K.; Zhang, T.; Lv, C.; Wang, H.; Zhao, G.
Deposited on : 2019-03-20
Resolution : 2.93 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:

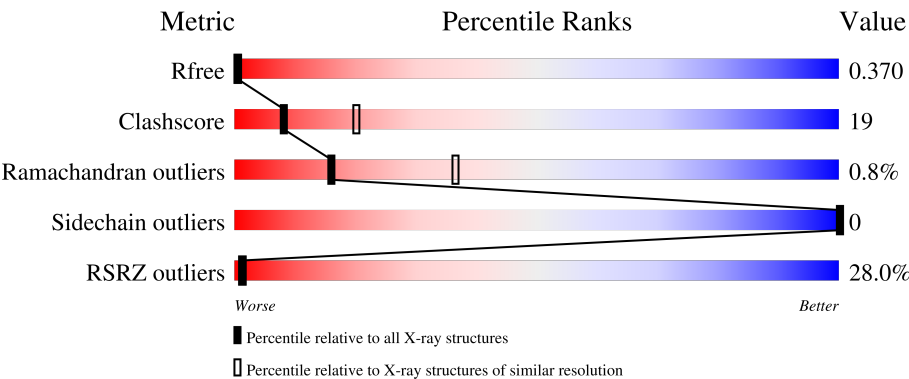
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	183	21% 63% 28% 6%
1	B	183	27% 55% 36% 6%
1	C	183	23% 56% 36% 6%
1	D	183	26% 60% 33% 6%
1	E	183	28% 63% 28% 6%

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Mol	Chain	Length	Quality of chain
1	F	183	25% 58% 34% 6%
1	G	183	32% 59% 34% 6%
1	H	183	25% 50% 42% 6%
1	I	183	27% 59% 34% 6%
1	J	183	27% 60% 33% 6%
1	K	183	25% 55% 38% 6%
1	L	183	31% 58% 35% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16956 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	B	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	C	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	D	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	E	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	F	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	G	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	H	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	I	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	J	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	K	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			
1	L	172	Total	C	N	O	S	0	0	0
			1413	887	248	270	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
A	160	LEU	ALA	conflict	UNP P02794
A	161	MET	PRO	conflict	UNP P02794
A	162	VAL	GLU	conflict	UNP P02794
A	163	GLY	SER	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	86	GLN	LYS	conflict	UNP P02794
B	160	LEU	ALA	conflict	UNP P02794
B	161	MET	PRO	conflict	UNP P02794
B	162	VAL	GLU	conflict	UNP P02794
B	163	GLY	SER	conflict	UNP P02794
C	86	GLN	LYS	conflict	UNP P02794
C	160	LEU	ALA	conflict	UNP P02794
C	161	MET	PRO	conflict	UNP P02794
C	162	VAL	GLU	conflict	UNP P02794
C	163	GLY	SER	conflict	UNP P02794
D	86	GLN	LYS	conflict	UNP P02794
D	160	LEU	ALA	conflict	UNP P02794
D	161	MET	PRO	conflict	UNP P02794
D	162	VAL	GLU	conflict	UNP P02794
D	163	GLY	SER	conflict	UNP P02794
E	86	GLN	LYS	conflict	UNP P02794
E	160	LEU	ALA	conflict	UNP P02794
E	161	MET	PRO	conflict	UNP P02794
E	162	VAL	GLU	conflict	UNP P02794
E	163	GLY	SER	conflict	UNP P02794
F	86	GLN	LYS	conflict	UNP P02794
F	160	LEU	ALA	conflict	UNP P02794
F	161	MET	PRO	conflict	UNP P02794
F	162	VAL	GLU	conflict	UNP P02794
F	163	GLY	SER	conflict	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
G	160	LEU	ALA	conflict	UNP P02794
G	161	MET	PRO	conflict	UNP P02794
G	162	VAL	GLU	conflict	UNP P02794
G	163	GLY	SER	conflict	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
H	160	LEU	ALA	conflict	UNP P02794
H	161	MET	PRO	conflict	UNP P02794
H	162	VAL	GLU	conflict	UNP P02794
H	163	GLY	SER	conflict	UNP P02794
I	86	GLN	LYS	conflict	UNP P02794
I	160	LEU	ALA	conflict	UNP P02794
I	161	MET	PRO	conflict	UNP P02794
I	162	VAL	GLU	conflict	UNP P02794
I	163	GLY	SER	conflict	UNP P02794
J	86	GLN	LYS	conflict	UNP P02794
J	160	LEU	ALA	conflict	UNP P02794

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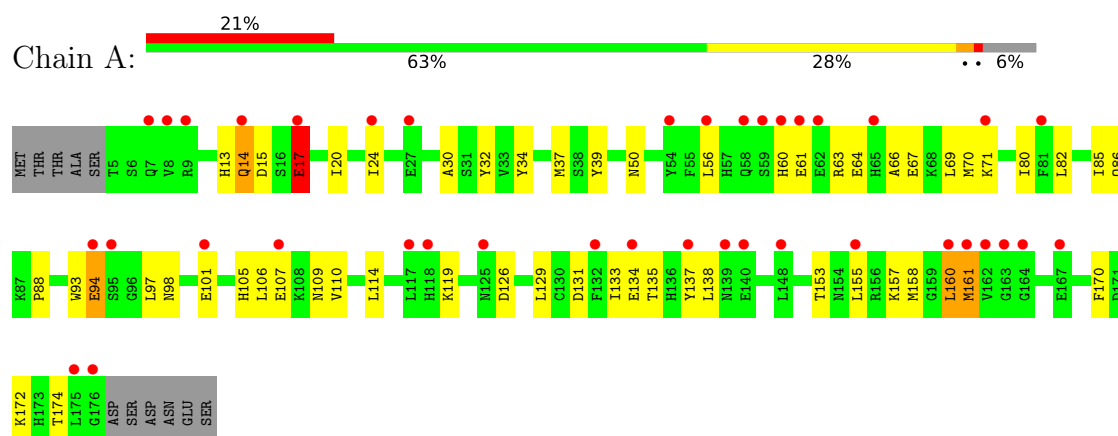
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Chain	Residue	Modelled	Actual	Comment	Reference
J	161	MET	PRO	conflict	UNP P02794
J	162	VAL	GLU	conflict	UNP P02794
J	163	GLY	SER	conflict	UNP P02794
K	86	GLN	LYS	conflict	UNP P02794
K	160	LEU	ALA	conflict	UNP P02794
K	161	MET	PRO	conflict	UNP P02794
K	162	VAL	GLU	conflict	UNP P02794
K	163	GLY	SER	conflict	UNP P02794
L	86	GLN	LYS	conflict	UNP P02794
L	160	LEU	ALA	conflict	UNP P02794
L	161	MET	PRO	conflict	UNP P02794
L	162	VAL	GLU	conflict	UNP P02794
L	163	GLY	SER	conflict	UNP P02794

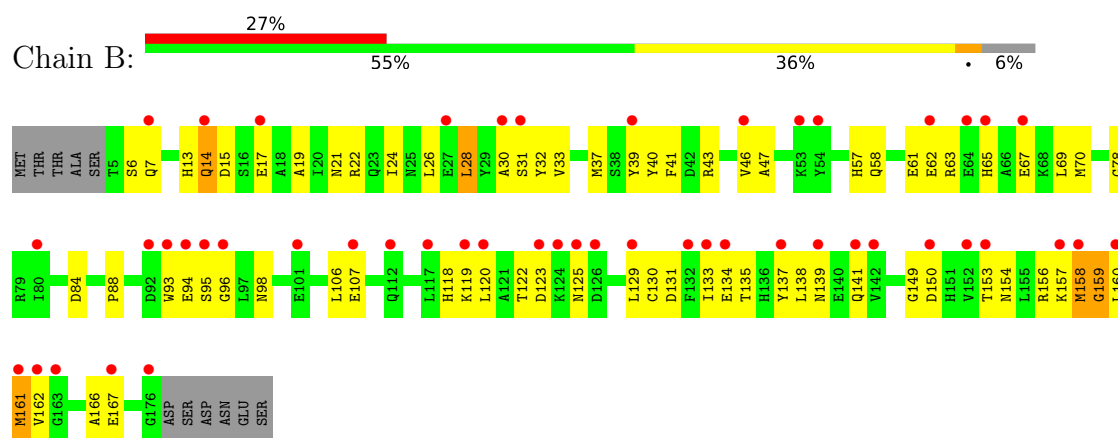
3 Residue-property plots [i](#)

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

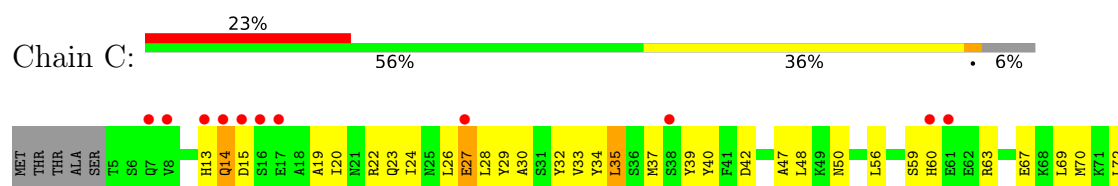
• Molecule 1: Ferritin heavy chain

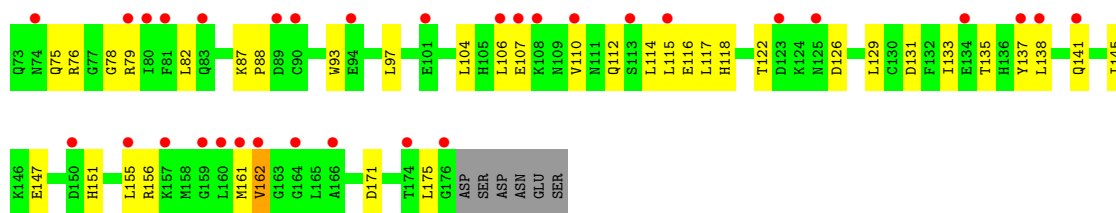


• Molecule 1: Ferritin heavy chain

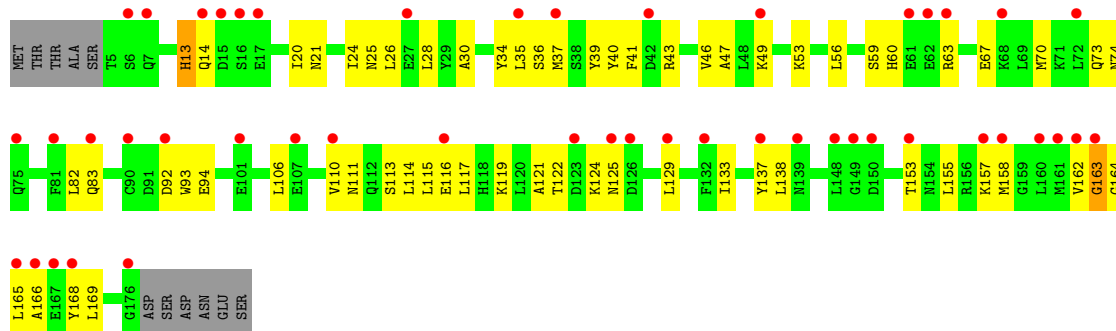


• Molecule 1: Ferritin heavy chain

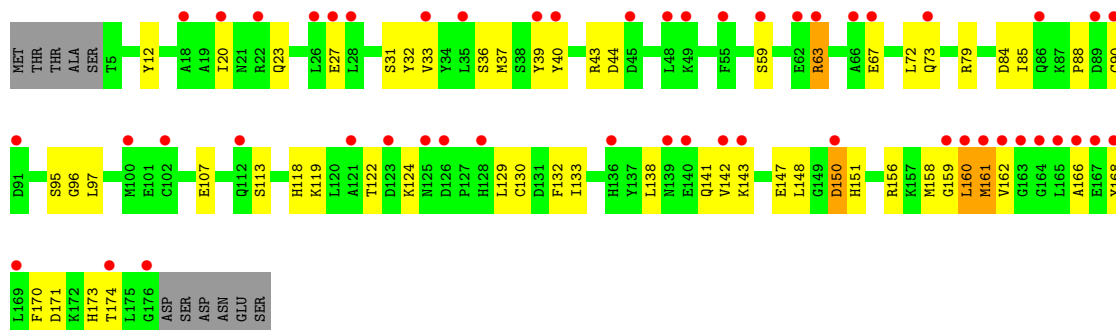




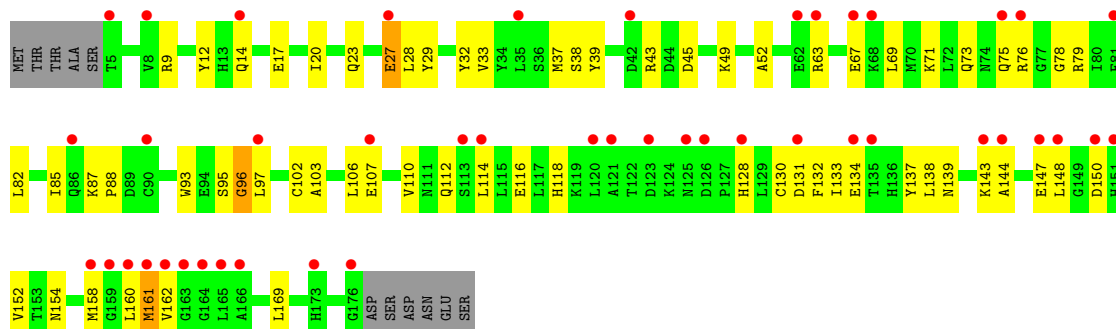
● Molecule 1: Ferritin heavy chain



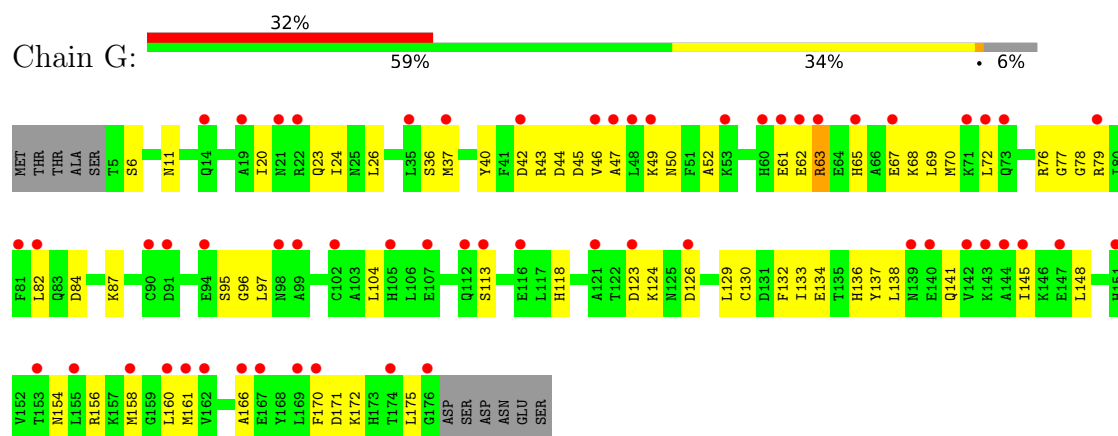
● Molecule 1: Ferritin heavy chain



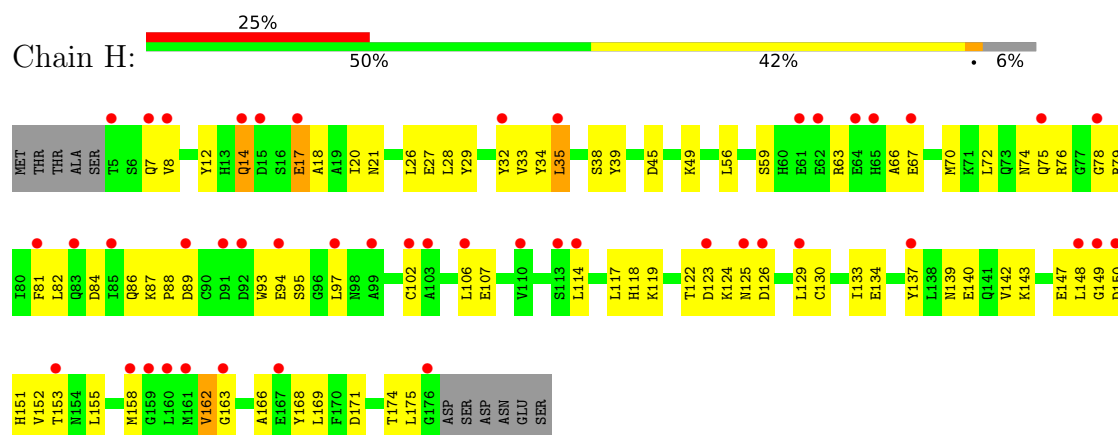
● Molecule 1: Ferritin heavy chain



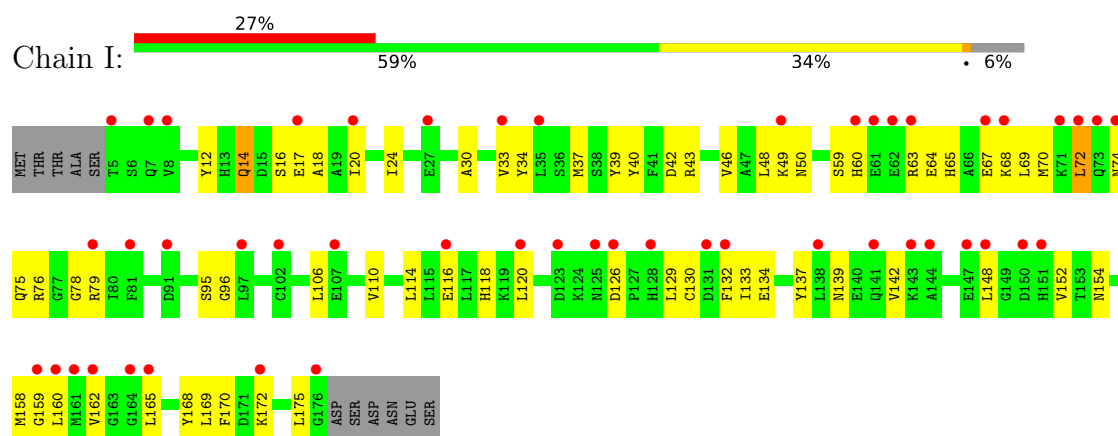
- Molecule 1: Ferritin heavy chain



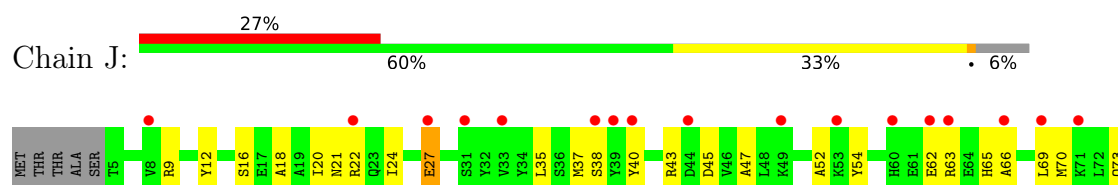
- Molecule 1: Ferritin heavy chain

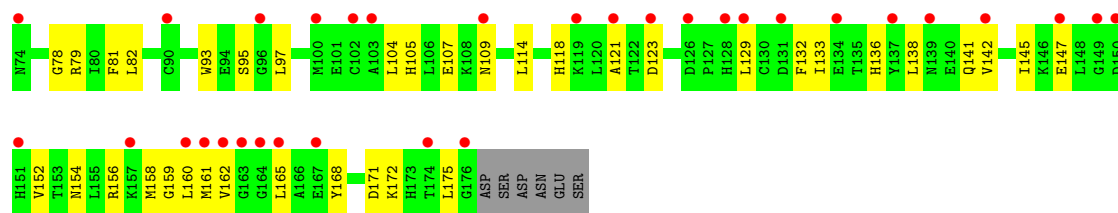


- Molecule 1: Ferritin heavy chain

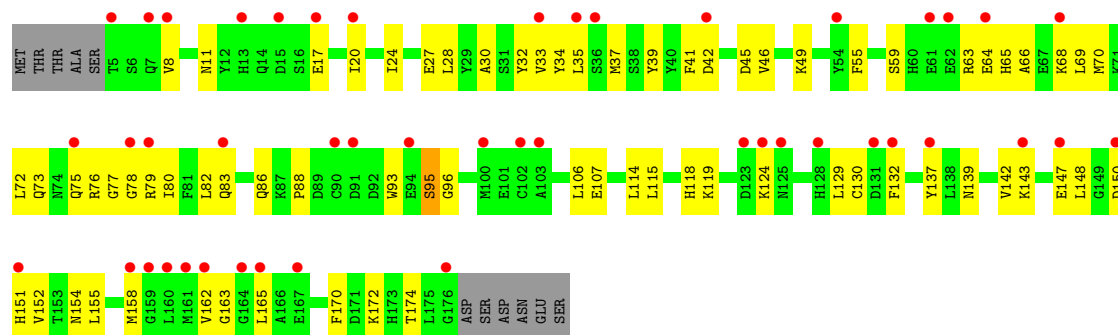


- Molecule 1: Ferritin heavy chain

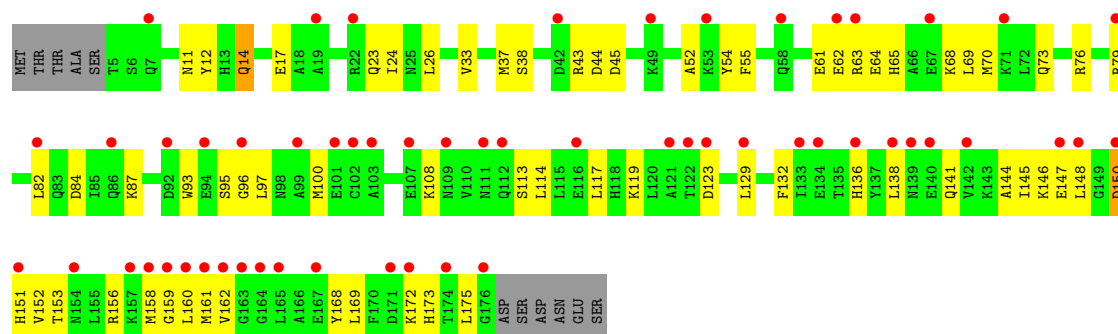




● Molecule 1: Ferritin heavy chain



● Molecule 1: Ferritin heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	219.17Å 219.17Å 147.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.01 – 2.93 107.01 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.5 (107.01-2.93) 98.0 (107.01-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.284 , 0.368 0.291 , 0.370	Depositor DCC
R_{free} test set	3859 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16956	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8143e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.48	0/1441	0.91	2/1940 (0.1%)
1	B	0.55	0/1441	0.95	4/1940 (0.2%)
1	C	0.58	0/1441	0.95	6/1940 (0.3%)
1	D	0.51	0/1441	0.86	4/1940 (0.2%)
1	E	0.53	0/1441	0.84	2/1940 (0.1%)
1	F	0.53	0/1441	0.95	5/1940 (0.3%)
1	G	0.50	0/1441	0.80	1/1940 (0.1%)
1	H	0.56	2/1441 (0.1%)	0.90	4/1940 (0.2%)
1	I	0.52	0/1441	0.94	7/1940 (0.4%)
1	J	0.55	1/1441 (0.1%)	0.82	0/1940
1	K	0.48	0/1441	0.90	7/1940 (0.4%)
1	L	0.52	0/1441	0.86	2/1940 (0.1%)
All	All	0.53	3/17292 (0.0%)	0.89	44/23280 (0.2%)

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	B	0	1
1	F	0	1
1	G	0	3
1	J	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	27	GLU	CB-CG	-6.62	1.32	1.52
1	H	17	GLU	CG-CD	-5.45	1.38	1.52
1	H	35	LEU	CG-CD1	5.01	1.69	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	GLU	CA-CB-CG	-9.12	95.86	114.10
1	F	96	GLY	CA-C-N	-7.67	108.66	121.92
1	F	96	GLY	C-N-CA	-7.67	108.66	121.92
1	L	150	ASP	CB-CA-C	-7.29	99.44	110.88
1	C	14	GLN	CA-CB-CG	-7.27	99.57	114.10
1	C	27	GLU	CA-CB-CG	-7.11	99.88	114.10
1	C	35	LEU	CA-CB-CG	6.93	140.55	116.30
1	E	150	ASP	CB-CA-C	-6.88	100.08	110.88
1	I	14	GLN	CA-CB-CG	6.82	127.73	114.10
1	B	14	GLN	N-CA-CB	-6.75	98.85	110.32
1	K	172	LYS	CA-CB-CG	-6.67	100.75	114.10
1	F	14	GLN	CA-CB-CG	6.61	127.32	114.10
1	H	17	GLU	CA-CB-CG	-6.60	100.90	114.10
1	I	116	GLU	CA-CB-CG	6.51	127.12	114.10
1	B	158	MET	CB-CG-SD	-6.47	93.29	112.70
1	C	115	LEU	CA-CB-CG	6.36	138.57	116.30
1	A	17	GLU	CB-CG-CD	6.29	123.29	112.60
1	C	35	LEU	CB-CA-C	-6.21	100.30	110.85
1	H	17	GLU	CB-CG-CD	6.00	122.80	112.60
1	D	13	HIS	CA-C-N	5.98	128.29	120.28
1	D	13	HIS	C-N-CA	5.98	128.29	120.28
1	G	63	ARG	CG-CD-NE	5.97	125.14	112.00
1	D	35	LEU	CA-CB-CG	5.89	136.91	116.30
1	K	83	GLN	CA-CB-CG	5.88	125.86	114.10
1	D	14	GLN	CB-CG-CD	-5.82	102.71	112.60
1	E	63	ARG	CG-CD-NE	5.73	124.62	112.00
1	I	72	LEU	CA-C-N	-5.68	113.05	120.44
1	I	72	LEU	C-N-CA	-5.68	113.05	120.44
1	I	116	GLU	CG-CD-OE2	-5.64	105.42	118.40
1	A	14	GLN	N-CA-CB	5.60	119.69	110.39
1	F	27	GLU	CG-CD-OE1	-5.60	105.52	118.40
1	B	125	ASN	N-CA-CB	-5.45	103.04	111.65
1	H	158	MET	CB-CG-SD	-5.44	96.38	112.70
1	K	75	GLN	N-CA-CB	-5.33	102.01	110.28
1	B	28	LEU	CA-CB-CG	5.32	134.93	116.30
1	H	14	GLN	N-CA-C	-5.26	106.12	112.54
1	K	124	LYS	CA-C-N	5.23	130.36	122.68
1	K	124	LYS	C-N-CA	5.23	130.36	122.68
1	I	116	GLU	CG-CD-OE1	5.19	130.33	118.40
1	K	75	GLN	CA-CB-CG	5.17	124.44	114.10
1	C	35	LEU	CB-CG-CD1	-5.09	95.43	110.70
1	K	95	SER	N-CA-C	5.08	115.90	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	72	LEU	CB-CG-CD2	-5.06	95.51	110.70
1	L	14	GLN	N-CA-CB	-5.06	101.71	110.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLU	Sidechain
1	B	138	LEU	Peptide
1	F	161	MET	Peptide
1	G	160	LEU	Peptide
1	G	161	MET	Peptide
1	G	61	GLU	Peptide
1	J	147	GLU	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	1413	0	1361	42	1
1	B	1413	0	1361	65	0
1	C	1413	0	1361	70	0
1	D	1413	0	1361	52	1
1	E	1413	0	1361	55	0
1	F	1413	0	1361	58	0
1	G	1413	0	1361	62	1
1	H	1413	0	1361	76	1
1	I	1413	0	1361	64	1
1	J	1413	0	1361	56	1
1	K	1413	0	1361	62	0
1	L	1413	0	1361	57	0
All	All	16956	0	16332	647	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 (647) 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:I:63:ARG:O	1:I:67:GLU:OE2	1.53	1.25
1:K:64:GLU:O	1:K:68:LYS:HD3	1.49	1.13
1:K:20:ILE:HD12	1:K:73:GLN:HG2	1.24	1.12
1:C:114:LEU:HD22	1:C:138:LEU:CD1	1.81	1.11
1:K:20:ILE:CD1	1:K:73:GLN:HG2	1.80	1.09
1:H:17:GLU:HG3	1:H:18:ALA:N	1.63	1.08
1:G:141:GLN:O	1:G:145:ILE:HD12	1.54	1.04
1:K:20:ILE:HD12	1:K:73:GLN:CG	1.88	1.03
1:C:114:LEU:HD22	1:C:138:LEU:HD11	1.04	1.02
1:C:114:LEU:CD2	1:C:138:LEU:HD11	1.92	1.00
1:L:147:GLU:O	1:L:150:ASP:OD2	1.81	0.97
1:K:64:GLU:HB3	1:K:68:LYS:HE2	1.47	0.95
1:A:98:ASN:HA	1:A:101:GLU:HG2	1.51	0.92
1:K:64:GLU:O	1:K:68:LYS:CD	2.17	0.92
1:I:74:ASN:HD22	1:J:43:ARG:HG2	1.35	0.91
1:I:17:GLU:HG3	1:I:18:ALA:N	1.85	0.89
1:C:24:ILE:O	1:C:28:LEU:CD2	2.21	0.89
1:L:150:ASP:OD1	1:L:151:HIS:CD2	2.27	0.88
1:K:20:ILE:CD1	1:K:73:GLN:CG	2.50	0.87
1:G:72:LEU:HD13	1:G:132:PHE:CD1	2.10	0.86
1:L:144:ALA:O	1:L:148:LEU:HD22	1.74	0.86
1:I:63:ARG:CZ	1:J:63:ARG:NH2	2.38	0.86
1:E:12:TYR:OH	1:E:73:GLN:NE2	2.08	0.85
1:L:14:GLN:HA	1:L:17:GLU:HG2	1.57	0.85
1:D:21:ASN:HA	1:D:24:ILE:HD12	1.58	0.84
1:H:32:TYR:CD2	1:H:88:PRO:HD3	2.13	0.84
1:K:139:ASN:HA	1:K:142:VAL:HG12	1.60	0.84
1:B:158:MET:HE1	1:B:166:ALA:HA	1.60	0.83
1:J:118:HIS:HB2	1:J:133:ILE:HD11	1.62	0.82
1:F:144:ALA:O	1:F:148:LEU:CD2	2.27	0.82
1:G:134:GLU:HA	1:G:138:LEU:HD12	1.61	0.82
1:C:97:LEU:HB2	1:C:155:LEU:HD22	1.62	0.81
1:I:63:ARG:NH2	1:J:63:ARG:NH2	2.28	0.81
1:B:96:GLY:HA3	1:B:167:GLU:OE1	1.80	0.81
1:F:144:ALA:O	1:F:148:LEU:HD22	1.79	0.80
1:I:110:VAL:O	1:I:114:LEU:HD12	1.82	0.80
1:E:118:HIS:CD2	1:E:133:ILE:HD11	2.17	0.79
1:G:72:LEU:HD13	1:G:132:PHE:CE1	2.19	0.78
1:K:20:ILE:HD11	1:K:73:GLN:CD	2.08	0.78
1:D:114:LEU:HD21	1:D:137:TYR:HB3	1.65	0.78
1:J:107:GLU:OE2	1:J:141:GLN:NE2	2.12	0.77
1:L:144:ALA:O	1:L:148:LEU:CD2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:O	1:A:109:ASN:ND2	2.16	0.76
1:G:72:LEU:HD13	1:G:132:PHE:CG	2.20	0.76
1:C:24:ILE:O	1:C:28:LEU:HD23	1.85	0.76
1:C:114:LEU:CD2	1:C:138:LEU:CD1	2.59	0.76
1:E:119:LYS:HA	1:E:122:THR:HG22	1.68	0.76
1:G:141:GLN:O	1:G:145:ILE:CD1	2.33	0.76
1:G:20:ILE:HG23	1:G:69:LEU:HD22	1.69	0.75
1:L:158:MET:O	1:L:160:LEU:N	2.20	0.75
1:C:161:MET:HG3	1:C:162:VAL:HG22	1.67	0.75
1:A:158:MET:HE1	1:A:170:PHE:HB2	1.70	0.73
1:C:114:LEU:HD11	1:C:137:TYR:HB3	1.70	0.73
1:K:20:ILE:CD1	1:K:73:GLN:CD	2.61	0.73
1:E:44:ASP:OD1	1:F:79:ARG:NH2	2.21	0.73
1:I:72:LEU:HD23	1:I:132:PHE:CE2	2.24	0.73
1:G:11:ASN:O	1:G:76:ARG:NH2	2.21	0.73
1:I:67:GLU:HA	1:I:70:MET:HE3	1.70	0.73
1:C:24:ILE:O	1:C:28:LEU:HD22	1.88	0.72
1:D:117:LEU:HD12	1:D:133:ILE:HG13	1.70	0.72
1:B:107:GLU:OE1	1:B:141:GLN:OE1	2.09	0.71
1:I:74:ASN:ND2	1:J:43:ARG:HG2	2.06	0.70
1:J:9:ARG:NH1	1:J:12:TYR:O	2.24	0.70
1:G:72:LEU:CD1	1:G:132:PHE:CD1	2.73	0.70
1:C:20:ILE:HD12	1:C:117:LEU:HD21	1.74	0.70
1:A:160:LEU:HA	1:A:161:MET:C	2.17	0.70
1:B:28:LEU:HA	1:B:31:SER:HB3	1.74	0.69
1:L:43:ARG:NH2	1:L:45:ASP:OD2	2.25	0.69
1:H:114:LEU:HD13	1:H:137:TYR:HB3	1.74	0.69
1:H:17:GLU:CG	1:H:18:ALA:N	2.51	0.69
1:H:162:VAL:HG12	1:H:163:GLY:H	1.57	0.69
1:I:78:GLY:C	1:I:79:ARG:HD2	2.18	0.68
1:D:41:PHE:HA	1:D:46:VAL:HG21	1.75	0.68
1:E:20:ILE:HD11	1:E:129:LEU:HD11	1.76	0.68
1:I:72:LEU:CD2	1:I:132:PHE:CD2	2.77	0.68
1:L:45:ASP:OD1	1:L:45:ASP:N	2.27	0.68
1:K:151:HIS:O	1:K:155:LEU:HD12	1.94	0.67
1:B:57:HIS:NE2	1:B:61:GLU:OE1	2.28	0.67
1:G:87:LYS:N	1:H:84:ASP:OD1	2.27	0.67
1:K:150:ASP:OD1	1:K:151:HIS:N	2.27	0.67
1:B:13:HIS:CE1	1:B:14:GLN:NE2	2.63	0.67
1:F:23:GLN:HG3	1:F:27:GLU:OE1	1.94	0.67
1:I:33:VAL:HG11	1:I:106:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:THR:OG1	1:J:168:TYR:OH	2.12	0.67
1:K:114:LEU:HD13	1:K:137:TYR:HB3	1.77	0.67
1:A:39:TYR:OH	1:B:67:GLU:HB2	1.95	0.66
1:G:43:ARG:HH11	1:H:79:ARG:NE	1.92	0.66
1:E:67:GLU:HB2	1:F:39:TYR:OH	1.94	0.66
1:J:12:TYR:OH	1:J:73:GLN:OE1	2.13	0.66
1:I:69:LEU:HG	1:I:137:TYR:OH	1.96	0.65
1:J:27:GLU:CD	1:J:27:GLU:N	2.54	0.65
1:D:153:THR:O	1:D:157:LYS:HG3	1.96	0.65
1:D:21:ASN:ND2	1:D:73:GLN:OE1	2.29	0.65
1:H:106:LEU:C	1:H:106:LEU:HD23	2.22	0.65
1:I:64:GLU:O	1:I:68:LYS:HG2	1.97	0.65
1:B:119:LYS:NZ	1:B:122:THR:HG21	2.12	0.65
1:J:27:GLU:CD	1:J:27:GLU:H	2.05	0.65
1:L:97:LEU:HD21	1:L:156:ARG:HG2	1.78	0.65
1:C:26:LEU:O	1:C:29:TYR:HB3	1.97	0.64
1:H:130:CYS:O	1:H:134:GLU:HG2	1.96	0.64
1:G:82:LEU:HB3	1:H:32:TYR:OH	1.97	0.64
1:B:94:GLU:O	1:B:98:ASN:HB3	1.97	0.64
1:K:27:GLU:HB2	1:K:66:ALA:HB2	1.79	0.64
1:H:21:ASN:HD21	1:H:81:PHE:HB2	1.61	0.64
1:B:158:MET:CE	1:B:166:ALA:HA	2.26	0.64
1:D:37:MET:HG2	1:D:93:TRP:CE2	2.33	0.63
1:H:75:GLN:HA	1:L:146:LYS:HD3	1.78	0.63
1:I:16:SER:O	1:I:20:ILE:HD12	1.99	0.63
1:I:34:TYR:HB2	1:I:59:SER:HB2	1.80	0.63
1:C:107:GLU:HA	1:C:110:VAL:HG12	1.80	0.63
1:H:7:GLN:HE22	1:L:153:THR:HG23	1.62	0.63
1:A:107:GLU:HA	1:A:110:VAL:HG12	1.81	0.63
1:F:154:ASN:O	1:F:158:MET:HG3	1.98	0.63
1:H:67:GLU:HA	1:H:70:MET:HE3	1.81	0.63
1:H:7:GLN:HE22	1:L:153:THR:CG2	2.11	0.63
1:K:34:TYR:HB2	1:K:59:SER:HB2	1.81	0.62
1:D:20:ILE:HG22	1:D:117:LEU:HD21	1.80	0.62
1:G:72:LEU:HD13	1:G:132:PHE:CD2	2.33	0.62
1:I:20:ILE:HD11	1:I:129:LEU:HD21	1.82	0.62
1:B:62:GLU:HA	1:B:65:HIS:HB2	1.82	0.62
1:B:123:ASP:OD1	1:H:123:ASP:CG	2.42	0.62
1:J:154:ASN:O	1:J:158:MET:HG3	1.99	0.62
1:I:70:MET:HE1	1:J:35:LEU:HD21	1.81	0.62
1:J:118:HIS:CB	1:J:133:ILE:HD11	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:O	1:A:98:ASN:HB3	2.00	0.61
1:G:126:ASP:OD2	1:G:129:LEU:HB2	2.00	0.61
1:B:129:LEU:HD23	1:B:129:LEU:O	1.99	0.61
1:H:118:HIS:NE2	1:H:130:CYS:HB3	2.14	0.61
1:J:82:LEU:HD12	1:J:82:LEU:H	1.65	0.61
1:G:72:LEU:HD13	1:G:132:PHE:CZ	2.35	0.61
1:C:114:LEU:HD23	1:C:114:LEU:O	1.99	0.61
1:L:168:TYR:HD1	1:L:169:LEU:HD23	1.63	0.61
1:K:170:PHE:CE2	1:K:174:THR:HG21	2.35	0.61
1:C:35:LEU:HD13	1:D:70:MET:HE1	1.82	0.61
1:I:148:LEU:O	1:I:152:VAL:HG12	2.01	0.61
1:H:139:ASN:HA	1:H:142:VAL:HG12	1.82	0.60
1:B:96:GLY:CA	1:B:167:GLU:OE1	2.49	0.60
1:C:60:HIS:HA	1:C:63:ARG:NH2	2.16	0.60
1:H:93:TRP:HZ3	1:H:102:CYS:HG	1.49	0.60
1:B:65:HIS:O	1:B:137:TYR:OH	2.16	0.60
1:J:78:GLY:O	1:J:79:ARG:HD3	2.02	0.59
1:H:35:LEU:HG	1:H:59:SER:OG	2.02	0.59
1:G:40:TYR:O	1:G:43:ARG:HG3	2.03	0.59
1:G:43:ARG:HB2	1:G:46:VAL:HG12	1.83	0.59
1:E:173:HIS:HB3	1:J:172:LYS:HD2	1.85	0.59
1:F:45:ASP:OD1	1:F:45:ASP:N	2.32	0.59
1:H:32:TYR:HE2	1:H:87:LYS:HA	1.66	0.59
1:C:87:LYS:HE3	1:C:88:PRO:O	2.03	0.59
1:E:158:MET:HE1	1:E:170:PHE:HB2	1.84	0.59
1:J:162:VAL:HG12	1:J:165:LEU:HD21	1.85	0.59
1:I:14:GLN:HA	1:I:17:GLU:HG2	1.85	0.58
1:L:150:ASP:CG	1:L:151:HIS:N	2.61	0.58
1:A:24:ILE:HD12	1:A:70:MET:HG2	1.85	0.58
1:H:162:VAL:HG12	1:H:163:GLY:N	2.19	0.58
1:J:38:SER:HB2	1:J:52:ALA:O	2.02	0.58
1:K:17:GLU:HG3	1:K:78:GLY:HA3	1.86	0.58
1:A:13:HIS:ND1	1:A:15:ASP:HB2	2.18	0.58
1:D:13:HIS:CD2	1:D:124:LYS:HD2	2.38	0.58
1:J:16:SER:O	1:J:20:ILE:HG12	2.04	0.58
1:I:139:ASN:HA	1:I:142:VAL:HG12	1.86	0.58
1:I:63:ARG:CZ	1:J:63:ARG:CZ	2.81	0.58
1:E:118:HIS:HD2	1:E:133:ILE:HD11	1.64	0.57
1:I:30:ALA:O	1:I:33:VAL:HG12	2.04	0.57
1:B:13:HIS:ND1	1:B:15:ASP:HB2	2.19	0.57
1:D:162:VAL:O	1:D:164:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:TYR:HE2	1:H:78:GLY:HA3	1.69	0.57
1:E:33:VAL:HG22	1:E:88:PRO:HB3	1.86	0.57
1:C:63:ARG:CD	1:D:63:ARG:CZ	2.83	0.57
1:A:14:GLN:O	1:A:17:GLU:HG3	2.05	0.57
1:E:147:GLU:HA	1:E:150:ASP:OD1	2.05	0.57
1:I:79:ARG:HD2	1:I:79:ARG:N	2.19	0.57
1:J:114:LEU:HD12	1:J:141:GLN:HG3	1.86	0.57
1:B:33:VAL:HG22	1:B:88:PRO:HB3	1.86	0.57
1:J:118:HIS:HB2	1:J:133:ILE:CD1	2.32	0.57
1:L:11:ASN:O	1:L:76:ARG:NH2	2.38	0.57
1:F:144:ALA:O	1:F:148:LEU:HD23	2.03	0.56
1:D:82:LEU:HD22	1:D:82:LEU:H	1.69	0.56
1:L:82:LEU:HD12	1:L:82:LEU:H	1.70	0.56
1:D:113:SER:HA	1:D:116:GLU:OE1	2.05	0.56
1:F:69:LEU:HG	1:F:137:TYR:OH	2.04	0.56
1:G:158:MET:HG3	1:G:166:ALA:HB1	1.88	0.56
1:G:77:GLY:O	1:G:79:ARG:NH1	2.39	0.56
1:L:148:LEU:HD22	1:L:148:LEU:H	1.71	0.56
1:I:17:GLU:HG3	1:I:18:ALA:H	1.66	0.56
1:C:67:GLU:HB3	1:D:39:TYR:OH	2.05	0.56
1:K:20:ILE:HD11	1:K:73:GLN:CG	2.33	0.56
1:H:93:TRP:HZ3	1:H:102:CYS:SG	2.29	0.56
1:K:69:LEU:HG	1:K:137:TYR:OH	2.06	0.56
1:A:30:ALA:HB1	1:A:106:LEU:HD21	1.88	0.56
1:B:14:GLN:HG2	1:B:15:ASP:N	2.21	0.55
1:E:97:LEU:HD21	1:E:156:ARG:HG2	1.88	0.55
1:G:72:LEU:HD13	1:G:132:PHE:CE2	2.41	0.55
1:A:133:ILE:HG22	1:A:138:LEU:HD11	1.88	0.55
1:E:23:GLN:OE1	1:E:113:SER:OG	2.25	0.55
1:G:79:ARG:HH21	1:H:45:ASP:CG	2.14	0.55
1:L:12:TYR:OH	1:L:73:GLN:OE1	2.25	0.55
1:H:32:TYR:CE2	1:H:88:PRO:HD3	2.42	0.55
1:H:171:ASP:HA	1:H:175:LEU:HD12	1.89	0.55
1:I:130:CYS:O	1:I:134:GLU:HG3	2.07	0.55
1:A:63:ARG:O	1:A:67:GLU:HG2	2.07	0.55
1:G:20:ILE:HD11	1:G:129:LEU:HD11	1.89	0.55
1:J:20:ILE:HG23	1:J:69:LEU:HD22	1.89	0.55
1:K:70:MET:HE3	1:K:82:LEU:HD21	1.87	0.55
1:B:107:GLU:CD	1:B:141:GLN:OE1	2.50	0.54
1:C:78:GLY:C	1:C:79:ARG:HD2	2.31	0.54
1:E:160:LEU:O	1:E:162:VAL:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LEU:HD22	1:F:137:TYR:HB3	1.89	0.54
1:G:72:LEU:CD1	1:G:132:PHE:CE1	2.88	0.54
1:J:118:HIS:CD2	1:J:133:ILE:HD11	2.42	0.54
1:E:133:ILE:HD12	1:E:138:LEU:HG	1.90	0.54
1:G:6:SER:HB2	1:G:79:ARG:HH22	1.72	0.54
1:H:78:GLY:C	1:H:79:ARG:HD3	2.31	0.54
1:K:65:HIS:O	1:K:137:TYR:OH	2.21	0.54
1:F:148:LEU:HD22	1:F:148:LEU:N	2.23	0.54
1:G:23:GLN:OE1	1:G:113:SER:HB3	2.07	0.54
1:I:72:LEU:CD2	1:I:132:PHE:CE2	2.90	0.54
1:J:121:ALA:HB2	1:J:129:LEU:HD23	1.90	0.54
1:B:67:GLU:HA	1:B:70:MET:HG3	1.89	0.54
1:E:95:SER:OG	1:E:97:LEU:N	2.41	0.54
1:H:32:TYR:CE2	1:H:87:LYS:HA	2.43	0.54
1:H:150:ASP:OD1	1:H:151:HIS:N	2.39	0.54
1:H:45:ASP:OD1	1:H:45:ASP:N	2.39	0.53
1:H:117:LEU:HG	1:H:133:ILE:HD11	1.89	0.53
1:K:33:VAL:HG23	1:K:88:PRO:HB3	1.90	0.53
1:B:131:ASP:HA	1:B:134:GLU:HG3	1.91	0.53
1:C:97:LEU:HD13	1:C:155:LEU:HB3	1.89	0.53
1:E:158:MET:HG3	1:E:166:ALA:HB1	1.90	0.53
1:F:71:LYS:O	1:F:75:GLN:HG3	2.09	0.53
1:B:30:ALA:HB1	1:B:106:LEU:HD21	1.91	0.53
1:C:70:MET:CE	1:C:82:LEU:HD11	2.39	0.53
1:J:62:GLU:HA	1:J:65:HIS:HB2	1.91	0.53
1:K:70:MET:HE2	1:K:80:ILE:HD13	1.91	0.53
1:L:150:ASP:CG	1:L:151:HIS:H	2.17	0.53
1:A:71:LYS:HG2	1:A:71:LYS:O	2.09	0.53
1:H:122:THR:O	1:H:125:ASN:ND2	2.42	0.53
1:L:148:LEU:HD22	1:L:148:LEU:N	2.23	0.53
1:G:50:ASN:HB2	1:G:171:ASP:OD2	2.08	0.53
1:H:21:ASN:ND2	1:H:81:PHE:HB2	2.23	0.53
1:B:17:GLU:OE1	1:B:78:GLY:HA2	2.09	0.52
1:C:13:HIS:ND1	1:C:15:ASP:HB2	2.24	0.52
1:F:12:TYR:HE2	1:F:78:GLY:HA3	1.74	0.52
1:F:28:LEU:HB3	1:F:85:ILE:HD12	1.91	0.52
1:A:131:ASP:O	1:A:135:THR:HG23	2.09	0.52
1:B:41:PHE:HA	1:B:46:VAL:HG21	1.90	0.52
1:D:155:LEU:HA	1:D:158:MET:HE2	1.91	0.52
1:K:34:TYR:OH	1:K:107:GLU:OE2	2.24	0.52
1:H:14:GLN:O	1:H:17:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:O	1:B:67:GLU:HG2	2.09	0.52
1:I:65:HIS:O	1:I:137:TYR:OH	2.23	0.52
1:I:33:VAL:HG11	1:I:106:LEU:CD1	2.39	0.52
1:B:159:GLY:O	1:B:160:LEU:HD13	2.10	0.52
1:H:29:TYR:O	1:H:33:VAL:HG13	2.09	0.52
1:I:42:ASP:OD1	1:I:49:LYS:NZ	2.40	0.52
1:B:58:GLN:O	1:B:62:GLU:HG3	2.10	0.51
1:B:137:TYR:O	1:B:141:GLN:HB2	2.10	0.51
1:A:153:THR:O	1:A:157:LYS:HG3	2.10	0.51
1:E:118:HIS:HB2	1:E:133:ILE:CD1	2.40	0.51
1:J:66:ALA:O	1:J:70:MET:HG3	2.10	0.51
1:C:30:ALA:CB	1:C:106:LEU:HD11	2.41	0.51
1:F:118:HIS:NE2	1:F:130:CYS:HB3	2.25	0.51
1:K:30:ALA:O	1:K:33:VAL:HG12	2.11	0.51
1:C:34:TYR:HB2	1:C:59:SER:HB2	1.92	0.51
1:H:107:GLU:HG3	1:H:148:LEU:HD12	1.92	0.51
1:H:147:GLU:O	1:H:150:ASP:OD1	2.27	0.51
1:K:45:ASP:OD1	1:L:79:ARG:NH2	2.43	0.51
1:C:137:TYR:O	1:C:141:GLN:HG2	2.11	0.51
1:I:64:GLU:HA	1:I:67:GLU:OE2	2.10	0.51
1:K:95:SER:OG	1:K:96:GLY:N	2.42	0.51
1:E:23:GLN:NE2	1:E:27:GLU:OE1	2.42	0.51
1:E:79:ARG:NE	1:F:43:ARG:HD2	2.26	0.51
1:E:84:ASP:OD1	1:F:87:LYS:N	2.43	0.51
1:F:97:LEU:HD11	1:F:152:VAL:HG13	1.92	0.51
1:G:154:ASN:O	1:G:158:MET:HE3	2.10	0.51
1:B:119:LYS:HZ1	1:B:122:THR:HG21	1.75	0.51
1:D:26:LEU:HD13	1:D:110:VAL:HG23	1.93	0.51
1:D:158:MET:HE3	1:D:166:ALA:HB1	1.92	0.51
1:K:154:ASN:O	1:K:158:MET:HG2	2.11	0.51
1:L:129:LEU:HD23	1:L:129:LEU:O	2.11	0.51
1:D:34:TYR:HB3	1:D:59:SER:HB2	1.91	0.50
1:H:163:GLY:O	1:H:166:ALA:HB3	2.11	0.50
1:L:24:ILE:HD13	1:L:70:MET:HG2	1.93	0.50
1:D:117:LEU:CD1	1:D:133:ILE:HG13	2.38	0.50
1:K:118:HIS:NE2	1:K:130:CYS:HB3	2.27	0.50
1:K:72:LEU:HD22	1:K:132:PHE:CE1	2.47	0.50
1:A:60:HIS:HA	1:A:63:ARG:NH2	2.27	0.50
1:B:6:SER:OG	1:B:7:GLN:N	2.45	0.50
1:G:46:VAL:HG13	1:G:47:ALA:H	1.76	0.50
1:K:20:ILE:HD11	1:K:73:GLN:HG2	1.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LEU:HD21	1:C:156:ARG:HG2	1.94	0.50
1:B:118:HIS:HA	1:B:133:ILE:HD11	1.94	0.50
1:D:129:LEU:O	1:D:129:LEU:HD23	2.12	0.50
1:F:106:LEU:C	1:F:106:LEU:HD23	2.36	0.50
1:C:56:LEU:HG	1:C:60:HIS:CD2	2.47	0.49
1:G:42:ASP:HB3	1:H:74:ASN:ND2	2.26	0.49
1:F:95:SER:OG	1:F:96:GLY:N	2.44	0.49
1:L:152:VAL:O	1:L:156:ARG:HG3	2.12	0.49
1:B:162:VAL:HG23	1:B:162:VAL:O	2.12	0.49
1:C:114:LEU:HD21	1:C:133:ILE:HG23	1.93	0.49
1:I:39:TYR:CD1	1:J:70:MET:HE3	2.47	0.49
1:I:168:TYR:CE1	1:I:172:LYS:HE3	2.47	0.49
1:K:147:GLU:O	1:K:150:ASP:OD1	2.31	0.49
1:C:70:MET:HE3	1:C:82:LEU:HD11	1.95	0.49
1:D:40:TYR:CE1	1:D:92:ASP:OD1	2.66	0.49
1:L:54:TYR:HB2	1:L:175:LEU:HD12	1.93	0.49
1:B:129:LEU:CD2	1:B:133:ILE:HD13	2.43	0.49
1:C:112:GLN:O	1:C:116:GLU:HG3	2.11	0.49
1:E:158:MET:HB2	1:J:165:LEU:HB3	1.95	0.49
1:G:172:LYS:HD2	1:L:173:HIS:HB3	1.93	0.49
1:F:133:ILE:HG22	1:F:138:LEU:HD13	1.95	0.49
1:E:72:LEU:HD13	1:E:132:PHE:CD1	2.48	0.49
1:C:47:ALA:O	1:C:48:LEU:HD23	2.12	0.49
1:C:107:GLU:HA	1:C:110:VAL:CG1	2.43	0.49
1:E:107:GLU:OE1	1:E:141:GLN:NE2	2.29	0.49
1:E:158:MET:CE	1:E:170:PHE:HB2	2.42	0.49
1:K:45:ASP:OD1	1:K:45:ASP:N	2.42	0.49
1:A:85:ILE:HD11	1:B:32:TYR:CZ	2.48	0.48
1:C:118:HIS:O	1:C:122:THR:HG23	2.12	0.48
1:I:72:LEU:HD21	1:I:132:PHE:CD2	2.47	0.48
1:J:138:LEU:O	1:J:142:VAL:HG23	2.13	0.48
1:A:32:TYR:CD2	1:A:88:PRO:HD3	2.48	0.48
1:G:72:LEU:CD1	1:G:132:PHE:CG	2.93	0.48
1:J:45:ASP:OD1	1:J:45:ASP:N	2.45	0.48
1:G:97:LEU:HD21	1:G:156:ARG:HG2	1.95	0.48
1:G:118:HIS:NE2	1:G:130:CYS:HB3	2.28	0.48
1:E:36:SER:HB2	1:F:82:LEU:HD12	1.96	0.48
1:F:33:VAL:HG21	1:F:106:LEU:HD13	1.96	0.48
1:B:130:CYS:O	1:B:134:GLU:HG3	2.14	0.48
1:G:170:PHE:CE1	1:G:175:LEU:HD13	2.48	0.48
1:C:33:VAL:HA	1:C:88:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ASP:HB3	1:D:74:ASN:HD22	1.79	0.48
1:C:69:LEU:HD13	1:C:137:TYR:OH	2.13	0.48
1:I:158:MET:HE1	1:I:170:PHE:HB2	1.95	0.48
1:D:165:LEU:HG	1:D:169:LEU:HG	1.96	0.48
1:L:37:MET:HG2	1:L:93:TRP:CE2	2.49	0.48
1:K:64:GLU:O	1:K:68:LYS:HD2	2.08	0.48
1:A:69:LEU:HD12	1:A:69:LEU:HA	1.64	0.48
1:B:120:LEU:HD11	1:H:124:LYS:NZ	2.29	0.48
1:D:119:LYS:HA	1:D:122:THR:HB	1.95	0.48
1:F:132:PHE:CE2	1:F:137:TYR:HE2	2.32	0.48
1:L:95:SER:OG	1:L:96:GLY:N	2.46	0.48
1:E:23:GLN:O	1:E:27:GLU:OE2	2.32	0.47
1:E:43:ARG:HE	1:F:79:ARG:HE	1.62	0.47
1:E:119:LYS:HA	1:E:122:THR:CG2	2.41	0.47
1:L:160:LEU:O	1:L:161:MET:HB2	2.13	0.47
1:C:37:MET:O	1:C:40:TYR:HB3	2.14	0.47
1:D:111:ASN:O	1:D:115:LEU:HG	2.15	0.47
1:J:105:HIS:O	1:J:109:ASN:ND2	2.47	0.47
1:C:82:LEU:HD22	1:D:36:SER:HB2	1.96	0.47
1:H:33:VAL:HG12	1:H:88:PRO:HG3	1.97	0.47
1:L:33:VAL:O	1:L:37:MET:HG3	2.14	0.47
1:D:46:VAL:HG23	1:D:47:ALA:N	2.30	0.47
1:H:8:VAL:HG13	1:L:145:ILE:HG22	1.97	0.47
1:I:162:VAL:HB	1:I:165:LEU:CD2	2.45	0.47
1:K:170:PHE:O	1:K:174:THR:HG22	2.14	0.47
1:F:37:MET:HG2	1:F:93:TRP:CE2	2.50	0.47
1:C:19:ALA:HA	1:C:22:ARG:CZ	2.45	0.47
1:F:28:LEU:HB3	1:F:85:ILE:CD1	2.45	0.47
1:H:20:ILE:HD13	1:H:117:LEU:HD21	1.96	0.47
1:H:78:GLY:O	1:H:79:ARG:HD3	2.15	0.47
1:K:41:PHE:HA	1:K:46:VAL:HG11	1.97	0.47
1:L:38:SER:OG	1:L:52:ALA:O	2.32	0.47
1:D:40:TYR:OH	1:D:94:GLU:O	2.32	0.46
1:G:49:LYS:O	1:G:52:ALA:HB3	2.15	0.46
1:H:119:LYS:HA	1:H:119:LYS:HD3	1.57	0.46
1:C:20:ILE:O	1:C:24:ILE:HG13	2.14	0.46
1:C:110:VAL:O	1:C:114:LEU:N	2.47	0.46
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.74	0.46
1:E:95:SER:OG	1:E:96:GLY:N	2.47	0.46
1:G:95:SER:OG	1:G:96:GLY:N	2.48	0.46
1:B:158:MET:O	1:B:159:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:HIS:O	1:B:122:THR:HG23	2.15	0.46
1:D:56:LEU:HG	1:D:60:HIS:CD2	2.50	0.46
1:F:20:ILE:HB	1:F:73:GLN:HE21	1.80	0.46
1:I:129:LEU:O	1:I:133:ILE:HG12	2.15	0.46
1:C:34:TYR:CB	1:C:59:SER:HB2	2.46	0.46
1:H:148:LEU:HA	1:H:148:LEU:HD23	1.64	0.46
1:I:14:GLN:CA	1:I:17:GLU:HG2	2.45	0.46
1:I:159:GLY:HA3	1:I:160:LEU:HA	1.80	0.46
1:J:104:LEU:HD11	1:J:145:ILE:HG23	1.97	0.46
1:A:67:GLU:HB2	1:B:39:TYR:OH	2.16	0.46
1:I:39:TYR:CE1	1:J:70:MET:HE3	2.51	0.46
1:L:43:ARG:HB3	1:L:45:ASP:OD1	2.16	0.46
1:A:107:GLU:HA	1:A:110:VAL:CG1	2.44	0.46
1:E:72:LEU:O	1:E:72:LEU:HG	2.13	0.46
1:G:50:ASN:HB2	1:G:171:ASP:CG	2.41	0.46
1:I:24:ILE:HD13	1:I:70:MET:HG2	1.97	0.46
1:K:42:ASP:OD1	1:K:49:LYS:NZ	2.49	0.46
1:A:119:LYS:HA	1:A:119:LYS:HD2	1.77	0.46
1:E:63:ARG:NE	1:F:63:ARG:CD	2.78	0.46
1:G:78:GLY:O	1:G:79:ARG:HD3	2.15	0.46
1:B:119:LYS:HZ2	1:B:122:THR:HG21	1.80	0.46
1:F:147:GLU:O	1:F:150:ASP:OD1	2.34	0.46
1:G:84:ASP:OD1	1:H:87:LYS:N	2.48	0.46
1:H:63:ARG:CZ	1:H:63:ARG:HB3	2.46	0.46
1:H:168:TYR:HD1	1:H:169:LEU:HD23	1.81	0.46
1:J:160:LEU:HB3	1:J:161:MET:H	1.63	0.46
1:K:33:VAL:HG11	1:K:106:LEU:HD22	1.98	0.46
1:L:144:ALA:O	1:L:148:LEU:HD23	2.13	0.46
1:A:80:ILE:HG22	1:A:82:LEU:HD12	1.98	0.46
1:C:161:MET:HG3	1:C:162:VAL:H	1.81	0.46
1:E:37:MET:O	1:E:40:TYR:HB3	2.15	0.46
1:I:14:GLN:O	1:I:17:GLU:HG2	2.15	0.46
1:J:37:MET:O	1:J:40:TYR:HB3	2.15	0.46
1:G:84:ASP:OD1	1:H:86:GLN:HA	2.15	0.45
1:K:72:LEU:HD21	1:K:129:LEU:HD13	1.98	0.45
1:D:34:TYR:CB	1:D:59:SER:HB2	2.47	0.45
1:H:27:GLU:HB2	1:H:66:ALA:HB2	1.98	0.45
1:H:93:TRP:O	1:H:95:SER:N	2.48	0.45
1:I:43:ARG:HH11	1:J:79:ARG:HD2	1.81	0.45
1:A:34:TYR:OH	1:A:107:GLU:OE2	2.24	0.45
1:B:131:ASP:O	1:B:135:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:O	1:C:162:VAL:HG23	2.16	0.45
1:F:93:TRP:HZ3	1:F:102:CYS:SG	2.40	0.45
1:G:123:ASP:O	1:G:124:LYS:HE3	2.16	0.45
1:I:76:ARG:HH22	1:I:126:ASP:CG	2.24	0.45
1:C:69:LEU:HD13	1:C:137:TYR:CZ	2.51	0.45
1:G:37:MET:O	1:G:40:TYR:HB3	2.16	0.45
1:I:120:LEU:HD12	1:I:120:LEU:HA	1.81	0.45
1:B:67:GLU:O	1:B:70:MET:HB2	2.16	0.45
1:D:163:GLY:O	1:D:166:ALA:HB3	2.16	0.45
1:G:24:ILE:HD13	1:G:70:MET:HG2	1.98	0.45
1:I:37:MET:O	1:I:40:TYR:HB3	2.17	0.45
1:G:20:ILE:CG2	1:G:69:LEU:HD22	2.44	0.45
1:A:134:GLU:HA	1:A:138:LEU:HD12	1.99	0.45
1:C:110:VAL:O	1:C:114:LEU:HB2	2.16	0.45
1:F:139:ASN:O	1:F:143:LYS:HG3	2.16	0.45
1:H:76:ARG:NH2	1:H:126:ASP:OD2	2.47	0.45
1:J:37:MET:HE2	1:J:93:TRP:CZ3	2.51	0.45
1:K:8:VAL:HG23	1:K:77:GLY:HA3	1.98	0.45
1:B:160:LEU:O	1:B:161:MET:HB2	2.15	0.45
1:C:171:ASP:HA	1:C:175:LEU:HD13	1.98	0.45
1:D:30:ALA:HB1	1:D:106:LEU:HD21	1.99	0.45
1:J:93:TRP:O	1:J:95:SER:N	2.43	0.45
1:K:139:ASN:HA	1:K:142:VAL:CG1	2.41	0.45
1:I:46:VAL:O	1:I:48:LEU:HD22	2.16	0.45
1:K:63:ARG:HD3	1:L:63:ARG:CZ	2.47	0.45
1:K:86:GLN:HA	1:L:84:ASP:OD1	2.17	0.45
1:C:13:HIS:ND1	1:C:14:GLN:HG2	2.32	0.45
1:C:13:HIS:CE1	1:C:15:ASP:HB2	2.52	0.45
1:E:118:HIS:HB2	1:E:133:ILE:HD11	1.99	0.45
1:G:68:LYS:HD3	1:G:136:HIS:ND1	2.32	0.45
1:H:140:GLU:OE1	1:H:143:LYS:HE3	2.16	0.45
1:J:37:MET:HG2	1:J:93:TRP:CE2	2.52	0.45
1:K:72:LEU:HD22	1:K:132:PHE:CD1	2.51	0.45
1:F:38:SER:HB2	1:F:52:ALA:O	2.17	0.44
1:G:26:LEU:HD12	1:G:26:LEU:HA	1.59	0.44
1:J:54:TYR:HB2	1:J:175:LEU:HD22	1.99	0.44
1:L:64:GLU:O	1:L:68:LYS:HG2	2.18	0.44
1:F:169:LEU:HD23	1:F:169:LEU:HA	1.77	0.44
1:L:62:GLU:HA	1:L:65:HIS:HB2	2.00	0.44
1:A:97:LEU:HB2	1:A:155:LEU:HD22	2.00	0.44
1:I:118:HIS:NE2	1:I:130:CYS:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:VAL:HG12	1:L:162:VAL:O	2.17	0.44
1:C:23:GLN:O	1:C:27:GLU:HG3	2.17	0.44
1:C:76:ARG:HH22	1:C:126:ASP:CG	2.25	0.44
1:J:132:PHE:O	1:J:136:HIS:HB2	2.18	0.44
1:J:168:TYR:O	1:J:171:ASP:HB3	2.17	0.44
1:K:39:TYR:CG	1:L:70:MET:HE2	2.52	0.44
1:F:37:MET:HE1	1:F:103:ALA:HB2	1.99	0.44
1:G:44:ASP:CG	1:H:79:ARG:HH22	2.20	0.44
1:H:28:LEU:HA	1:H:28:LEU:HD23	1.76	0.44
1:H:148:LEU:O	1:H:152:VAL:HG23	2.18	0.44
1:B:13:HIS:CE1	1:B:14:GLN:CD	2.96	0.44
1:C:63:ARG:HD2	1:D:63:ARG:CZ	2.47	0.44
1:G:43:ARG:HH11	1:H:79:ARG:HE	1.60	0.44
1:H:89:ASP:OD1	1:H:89:ASP:N	2.51	0.44
1:C:161:MET:HG3	1:C:162:VAL:N	2.33	0.44
1:I:169:LEU:HA	1:I:169:LEU:HD23	1.71	0.44
1:B:41:PHE:HA	1:B:46:VAL:CG2	2.47	0.44
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.84	0.44
1:I:50:ASN:HB3	1:I:175:LEU:O	2.18	0.44
1:I:63:ARG:NH2	1:J:63:ARG:HH22	2.12	0.44
1:D:49:LYS:HD2	1:D:49:LYS:N	2.33	0.43
1:K:79:ARG:HH22	1:L:44:ASP:CG	2.26	0.43
1:F:9:ARG:HH22	1:F:17:GLU:CD	2.27	0.43
1:F:69:LEU:HD23	1:F:69:LEU:HA	1.80	0.43
1:A:114:LEU:HD13	1:A:137:TYR:HB3	2.00	0.43
1:J:152:VAL:HG12	1:J:156:ARG:HD2	2.01	0.43
1:K:34:TYR:CB	1:K:59:SER:HB2	2.47	0.43
1:A:56:LEU:HG	1:A:60:HIS:CD2	2.53	0.43
1:D:162:VAL:HG22	1:D:165:LEU:HB3	2.00	0.43
1:F:148:LEU:HD22	1:F:148:LEU:H	1.83	0.43
1:G:148:LEU:HD13	1:G:148:LEU:HA	1.74	0.43
1:K:107:GLU:HG3	1:K:148:LEU:HD12	2.01	0.43
1:L:55:PHE:CZ	1:L:100:MET:HE2	2.54	0.43
1:A:61:GLU:HA	1:A:64:GLU:HB3	2.01	0.43
1:A:126:ASP:OD2	1:A:129:LEU:HB2	2.18	0.43
1:B:157:LYS:C	1:B:159:GLY:H	2.26	0.43
1:C:72:LEU:HA	1:C:75:GLN:HB2	2.00	0.43
1:E:124:LYS:HA	1:E:124:LYS:HD3	1.87	0.43
1:F:112:GLN:O	1:F:116:GLU:HG3	2.18	0.43
1:G:145:ILE:HD12	1:G:145:ILE:H	1.83	0.43
1:J:20:ILE:O	1:J:24:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LEU:HA	1:D:28:LEU:HD23	1.74	0.43
1:H:56:LEU:HD12	1:H:56:LEU:HA	1.84	0.43
1:I:69:LEU:HD23	1:I:69:LEU:HA	1.85	0.43
1:I:95:SER:OG	1:I:96:GLY:N	2.51	0.43
1:K:11:ASN:O	1:K:76:ARG:NH2	2.51	0.43
1:K:119:LYS:HD2	1:K:119:LYS:HA	1.46	0.43
1:K:148:LEU:HD23	1:K:148:LEU:HA	1.59	0.43
1:L:61:GLU:HA	1:L:64:GLU:HB3	2.00	0.43
1:A:66:ALA:O	1:A:70:MET:HG3	2.18	0.43
1:A:161:MET:C	1:A:161:MET:HE3	2.44	0.43
1:C:32:TYR:CD2	1:C:88:PRO:HD3	2.53	0.43
1:H:26:LEU:HD23	1:H:26:LEU:HA	1.63	0.43
1:H:97:LEU:HD13	1:H:155:LEU:HB2	1.99	0.43
1:L:23:GLN:OE1	1:L:113:SER:OG	2.35	0.43
1:E:88:PRO:C	1:E:90:CYS:H	2.26	0.43
1:G:44:ASP:O	1:L:153:THR:HG21	2.18	0.43
1:G:65:HIS:O	1:G:137:TYR:OH	2.30	0.43
1:J:97:LEU:HD21	1:J:156:ARG:HG3	2.00	0.43
1:B:40:TYR:O	1:B:43:ARG:HG3	2.19	0.43
1:B:159:GLY:C	1:B:160:LEU:HD22	2.44	0.43
1:E:39:TYR:OH	1:F:67:GLU:HB2	2.19	0.43
1:K:143:LYS:HB2	1:K:143:LYS:HE3	1.70	0.43
1:L:132:PHE:O	1:L:136:HIS:HB2	2.19	0.43
1:C:28:LEU:HD22	1:C:28:LEU:H	1.84	0.43
1:C:63:ARG:CZ	1:D:63:ARG:HD2	2.48	0.43
1:E:148:LEU:HD13	1:E:148:LEU:HA	1.85	0.42
1:G:129:LEU:HD23	1:G:133:ILE:HG12	2.01	0.42
1:H:106:LEU:C	1:H:106:LEU:CD2	2.91	0.42
1:K:8:VAL:HG23	1:K:77:GLY:CA	2.48	0.42
1:L:108:LYS:HG3	1:L:145:ILE:HD12	2.01	0.42
1:B:26:LEU:HD12	1:B:26:LEU:HA	1.87	0.42
1:C:50:ASN:HB2	1:C:171:ASP:OD1	2.19	0.42
1:D:165:LEU:HD21	1:D:169:LEU:CD1	2.50	0.42
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.85	0.42
1:B:157:LYS:HB3	1:B:157:LYS:HE2	1.81	0.42
1:C:50:ASN:HB3	1:C:175:LEU:HB2	2.01	0.42
1:E:36:SER:HB2	1:F:82:LEU:CD1	2.49	0.42
1:H:34:TYR:OH	1:H:107:GLU:OE1	2.36	0.42
1:I:154:ASN:O	1:I:158:MET:HG3	2.19	0.42
1:L:114:LEU:CD1	1:L:141:GLN:HG3	2.49	0.42
1:C:39:TYR:OH	1:D:67:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:LYS:HD2	1:H:49:LYS:HA	1.80	0.42
1:B:69:LEU:HD21	1:B:137:TYR:CE2	2.55	0.42
1:G:62:GLU:HA	1:G:65:HIS:HB2	2.02	0.42
1:I:168:TYR:CE1	1:I:172:LYS:CE	3.02	0.42
1:J:21:ASN:ND2	1:J:81:PHE:HB2	2.35	0.42
1:K:37:MET:HE3	1:K:55:PHE:CD2	2.53	0.42
1:L:117:LEU:HA	1:L:117:LEU:HD12	1.81	0.42
1:B:46:VAL:HG23	1:B:47:ALA:N	2.35	0.42
1:B:118:HIS:CE1	1:B:119:LYS:HZ2	2.38	0.42
1:C:30:ALA:HB1	1:C:106:LEU:HD11	2.01	0.42
1:D:49:LYS:HD2	1:D:49:LYS:H	1.84	0.42
1:E:32:TYR:CE1	1:F:82:LEU:HD13	2.55	0.42
1:E:151:HIS:ND1	1:E:170:PHE:HZ	2.18	0.42
1:F:160:LEU:HB3	1:F:161:MET:H	1.72	0.42
1:H:72:LEU:HD21	1:H:129:LEU:HD13	2.01	0.42
1:H:124:LYS:HA	1:H:124:LYS:HD3	1.84	0.42
1:I:63:ARG:C	1:I:67:GLU:OE2	2.48	0.42
1:B:120:LEU:HD11	1:H:124:LYS:HZ1	1.85	0.42
1:C:37:MET:HA	1:C:93:TRP:CD1	2.55	0.42
1:D:20:ILE:O	1:D:24:ILE:HG13	2.20	0.42
1:F:93:TRP:O	1:F:95:SER:N	2.47	0.42
1:F:130:CYS:O	1:F:134:GLU:HG2	2.19	0.42
1:G:104:LEU:CD1	1:G:145:ILE:HG23	2.50	0.42
1:K:162:VAL:HG12	1:K:165:LEU:HD23	2.01	0.42
1:B:37:MET:HE2	1:B:93:TRP:CZ3	2.55	0.42
1:D:157:LYS:HB3	1:D:157:LYS:HE2	1.65	0.42
1:E:85:ILE:HD11	1:F:32:TYR:CZ	2.55	0.42
1:H:21:ASN:HD21	1:H:81:PHE:CB	2.31	0.42
1:I:168:TYR:CZ	1:I:172:LYS:HD2	2.55	0.42
1:J:138:LEU:HD23	1:J:138:LEU:HA	1.85	0.42
1:B:21:ASN:HA	1:B:24:ILE:HD12	2.01	0.42
1:B:149:GLY:O	1:B:153:THR:HG23	2.20	0.41
1:E:138:LEU:O	1:E:142:VAL:HG23	2.20	0.41
1:F:107:GLU:HA	1:F:110:VAL:HG22	2.00	0.41
1:G:63:ARG:NH2	1:H:63:ARG:NH2	2.68	0.41
1:H:149:GLY:O	1:H:153:THR:HG23	2.20	0.41
1:I:12:TYR:HB2	1:I:76:ARG:HE	1.85	0.41
1:E:43:ARG:HE	1:F:79:ARG:NE	2.17	0.41
1:F:49:LYS:HD2	1:F:49:LYS:HA	1.65	0.41
1:F:131:ASP:OD2	1:F:131:ASP:C	2.63	0.41
1:A:30:ALA:CB	1:A:106:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASP:O	1:B:154:ASN:HB2	2.20	0.41
1:B:156:ARG:HE	1:B:156:ARG:HB3	1.69	0.41
1:C:131:ASP:OD2	1:C:135:THR:HG23	2.20	0.41
1:E:63:ARG:HD3	1:F:63:ARG:CZ	2.50	0.41
1:I:43:ARG:NH1	1:J:79:ARG:HD2	2.35	0.41
1:K:139:ASN:CA	1:K:142:VAL:HG12	2.41	0.41
1:B:19:ALA:HA	1:B:22:ARG:CZ	2.51	0.41
1:C:20:ILE:CD1	1:C:117:LEU:HD21	2.47	0.41
1:F:76:ARG:NH2	1:F:128:HIS:HB3	2.35	0.41
1:L:172:LYS:HA	1:L:172:LYS:HD3	1.89	0.41
1:A:24:ILE:HD13	1:A:69:LEU:HB3	2.03	0.41
1:F:33:VAL:HG12	1:F:88:PRO:HG3	2.01	0.41
1:G:67:GLU:HB3	1:H:39:TYR:OH	2.21	0.41
1:A:20:ILE:O	1:A:24:ILE:HG12	2.20	0.41
1:A:86:GLN:HA	1:B:84:ASP:OD1	2.20	0.41
1:A:155:LEU:HD23	1:A:155:LEU:O	2.20	0.41
1:B:93:TRP:O	1:B:94:GLU:C	2.62	0.41
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.88	0.41
1:F:9:ARG:NH2	1:F:17:GLU:OE1	2.48	0.41
1:I:106:LEU:C	1:I:106:LEU:HD23	2.45	0.41
1:J:118:HIS:CG	1:J:133:ILE:HD11	2.55	0.41
1:A:50:ASN:HD22	1:A:172:LYS:HA	1.86	0.41
1:C:20:ILE:HD11	1:C:129:LEU:HD11	2.02	0.41
1:D:53:LYS:HA	1:D:53:LYS:HD3	1.93	0.41
1:D:125:ASN:HD22	1:D:125:ASN:HA	1.64	0.41
1:E:168:TYR:O	1:E:171:ASP:HB3	2.21	0.41
1:L:26:LEU:HD12	1:L:26:LEU:HA	1.80	0.41
1:E:143:LYS:HE2	1:I:75:GLN:OE1	2.21	0.41
1:G:36:SER:HB2	1:H:82:LEU:HD12	2.03	0.41
1:G:158:MET:HE2	1:G:158:MET:HB3	1.90	0.41
1:I:60:HIS:O	1:I:63:ARG:HB3	2.21	0.41
1:K:32:TYR:CD2	1:K:88:PRO:HD3	2.56	0.41
1:L:69:LEU:HD23	1:L:69:LEU:HA	1.83	0.41
1:A:82:LEU:HD23	1:B:32:TYR:CE1	2.56	0.41
1:B:95:SER:OG	1:B:96:GLY:N	2.53	0.41
1:B:161:MET:HE3	1:B:161:MET:HA	2.02	0.41
1:D:117:LEU:C	1:D:117:LEU:HD13	2.45	0.41
1:E:170:PHE:HA	1:J:168:TYR:OH	2.21	0.41
1:G:44:ASP:HB3	1:L:146:LYS:HE2	2.03	0.41
1:G:45:ASP:HA	1:L:153:THR:HG21	2.03	0.41
1:H:168:TYR:O	1:H:171:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:ALA:O	1:J:22:ARG:HG2	2.21	0.41
1:L:119:LYS:O	1:L:123:ASP:HB2	2.21	0.41
1:C:131:ASP:O	1:C:135:THR:HG23	2.21	0.41
1:D:121:ALA:HB2	1:D:129:LEU:HD13	2.02	0.41
1:E:31:SER:O	1:E:59:SER:HB2	2.21	0.41
1:F:150:ASP:OD1	1:F:150:ASP:N	2.53	0.41
1:C:147:GLU:HG2	1:C:151:HIS:NE2	2.36	0.40
1:D:25:ASN:HD22	1:D:83:GLN:HB2	1.85	0.40
1:E:130:CYS:O	1:E:133:ILE:HG13	2.21	0.40
1:J:133:ILE:HG21	1:J:133:ILE:HD13	1.69	0.40
1:K:37:MET:HG3	1:K:93:TRP:CE2	2.56	0.40
1:C:104:LEU:CD1	1:C:145:ILE:HG23	2.51	0.40
1:G:133:ILE:HD13	1:G:133:ILE:HA	1.87	0.40
1:L:141:GLN:O	1:L:145:ILE:HG12	2.21	0.40
1:D:40:TYR:CD1	1:D:43:ARG:HD3	2.56	0.40
1:E:150:ASP:HB3	1:J:47:ALA:HB1	2.02	0.40
1:E:159:GLY:O	1:E:161:MET:N	2.54	0.40
1:K:35:LEU:HD23	1:K:35:LEU:HA	1.63	0.40
1:K:148:LEU:O	1:K:152:VAL:HG23	2.22	0.40
1:L:138:LEU:HD23	1:L:138:LEU:HA	1.84	0.40
1:A:30:ALA:HA	1:A:106:LEU:HD11	2.04	0.40
1:A:37:MET:HA	1:A:93:TRP:CD1	2.56	0.40
1:E:32:TYR:CZ	1:F:82:LEU:HD13	2.57	0.40
1:E:118:HIS:CG	1:E:133:ILE:HD11	2.54	0.40
1:F:29:TYR:O	1:F:33:VAL:HG13	2.20	0.40
1:I:20:ILE:HG23	1:I:69:LEU:HD22	2.03	0.40
1:I:69:LEU:HG	1:I:137:TYR:CZ	2.56	0.40
1:K:24:ILE:O	1:K:28:LEU:HD23	2.22	0.40
1:K:115:LEU:HD23	1:K:115:LEU:HA	1.89	0.40
1:D:40:TYR:HD1	1:D:43:ARG:HD3	1.86	0.40
1:H:38:SER:OG	1:H:56:LEU:HB2	2.22	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)
1:G:124:LYS:NZ	1:J:123:ASP:O[3_555]	1.88	0.32
1:A:174:THR:OG1	1:I:168:TYR:OH[6_554]	2.05	0.15
1:D:168:TYR:OH	1:H:174:THR:OG1[3_454]	2.15	0.05

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	170/183 (93%)	161 (95%)	6 (4%)	3 (2%)	6	19
1	B	170/183 (93%)	155 (91%)	12 (7%)	3 (2%)	6	19
1	C	170/183 (93%)	159 (94%)	10 (6%)	1 (1%)	21	45
1	D	170/183 (93%)	159 (94%)	10 (6%)	1 (1%)	21	45
1	E	170/183 (93%)	163 (96%)	5 (3%)	2 (1%)	10	27
1	F	170/183 (93%)	161 (95%)	8 (5%)	1 (1%)	21	45
1	G	170/183 (93%)	161 (95%)	9 (5%)	0	100	100
1	H	170/183 (93%)	161 (95%)	7 (4%)	2 (1%)	10	27
1	I	170/183 (93%)	163 (96%)	7 (4%)	0	100	100
1	J	170/183 (93%)	164 (96%)	5 (3%)	1 (1%)	21	45
1	K	170/183 (93%)	165 (97%)	4 (2%)	1 (1%)	21	45
1	L	170/183 (93%)	160 (94%)	8 (5%)	2 (1%)	10	27
All	All	2040/2196 (93%)	1932 (95%)	91 (4%)	17 (1%)	16	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	ASN
1	C	162	VAL
1	D	163	GLY
1	E	160	LEU
1	E	161	MET
1	H	94	GLU
1	K	163	GLY
1	A	94	GLU
1	A	161	MET
1	F	162	VAL
1	H	162	VAL
1	L	159	GLY

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Mol	Chain	Res	Type
1	B	161	MET
1	J	159	GLY
1	A	160	LEU
1	B	159	GLY
1	L	87	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	153/163 (94%)	153 (100%)	0	100	100
1	B	153/163 (94%)	153 (100%)	0	100	100
1	C	153/163 (94%)	153 (100%)	0	100	100
1	D	153/163 (94%)	153 (100%)	0	100	100
1	E	153/163 (94%)	153 (100%)	0	100	100
1	F	153/163 (94%)	153 (100%)	0	100	100
1	G	153/163 (94%)	153 (100%)	0	100	100
1	H	153/163 (94%)	153 (100%)	0	100	100
1	I	153/163 (94%)	153 (100%)	0	100	100
1	J	153/163 (94%)	153 (100%)	0	100	100
1	K	153/163 (94%)	153 (100%)	0	100	100
1	L	153/163 (94%)	153 (100%)	0	100	100
All	All	1836/1956 (94%)	1836 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	11	ASN
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	141	GLN
1	B	151	HIS
1	C	65	HIS
1	C	75	GLN
1	C	98	ASN
1	C	125	ASN
1	C	141	GLN
1	D	14	GLN
1	D	25	ASN
1	D	58	GLN
1	D	118	HIS
1	D	125	ASN
1	D	141	GLN
1	E	11	ASN
1	E	73	GLN
1	E	98	ASN
1	F	23	GLN
1	F	25	ASN
1	F	73	GLN
1	F	74	ASN
1	F	136	HIS
1	G	21	ASN
1	G	65	HIS
1	G	73	GLN
1	G	83	GLN
1	G	105	HIS
1	G	154	ASN
1	H	7	GLN
1	H	11	ASN
1	H	58	GLN
1	H	73	GLN
1	H	125	ASN
1	H	136	HIS
1	I	74	ASN
1	I	86	GLN
1	I	111	ASN
1	I	141	GLN
1	J	25	ASN
1	J	57	HIS
1	J	151	HIS
1	K	11	ASN
1	K	109	ASN

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Mol	Chain	Res	Type
1	L	7	GLN
1	L	57	HIS
1	L	83	GLN
1	L	151	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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	172/183 (93%)	1.33	39 (22%) 2 2	46, 65, 105, 157	0
1	B	172/183 (93%)	1.49	49 (28%) 1 1	41, 66, 105, 161	0
1	C	172/183 (93%)	1.39	43 (25%) 2 1	44, 65, 101, 149	0
1	D	172/183 (93%)	1.50	47 (27%) 1 1	45, 65, 100, 147	0
1	E	172/183 (93%)	1.56	51 (29%) 1 1	41, 63, 103, 136	0
1	F	172/183 (93%)	1.48	45 (26%) 1 1	40, 66, 108, 137	0
1	G	172/183 (93%)	1.65	58 (33%) 1 1	41, 64, 93, 142	0
1	H	172/183 (93%)	1.61	46 (26%) 1 1	39, 66, 103, 143	0
1	I	172/183 (93%)	1.57	49 (28%) 1 1	38, 66, 103, 140	0
1	J	172/183 (93%)	1.50	49 (28%) 1 1	40, 66, 98, 140	0
1	K	172/183 (93%)	1.56	46 (26%) 1 1	46, 65, 98, 155	0
1	L	172/183 (93%)	1.71	56 (32%) 1 1	39, 67, 97, 148	0
All	All	2064/2196 (93%)	1.53	578 (28%) 1 1	38, 65, 103, 161	0

All (578) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	150	ASP	8.0
1	D	7	GLN	7.9
1	L	96	GLY	7.8
1	F	150	ASP	7.1
1	L	150	ASP	7.1
1	H	125	ASN	7.0
1	K	160	LEU	6.1
1	H	14	GLN	6.0
1	K	162	VAL	6.0
1	D	176	GLY	5.8
1	E	27	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	160	LEU	5.7
1	H	35	LEU	5.7
1	G	123	ASP	5.7
1	I	102	CYS	5.6
1	K	8	VAL	5.6
1	G	73	GLN	5.6
1	H	8	VAL	5.5
1	K	102	CYS	5.4
1	K	150	ASP	5.4
1	J	162	VAL	5.4
1	H	32	TYR	5.4
1	C	176	GLY	5.3
1	I	107	GLU	5.3
1	K	83	GLN	5.3
1	D	83	GLN	5.3
1	A	176	GLY	5.3
1	B	176	GLY	5.3
1	K	125	ASN	5.2
1	J	150	ASP	5.2
1	A	107	GLU	5.2
1	D	17	GLU	5.2
1	L	162	VAL	5.1
1	B	158	MET	5.1
1	I	8	VAL	5.0
1	J	165	LEU	5.0
1	F	126	ASP	5.0
1	E	139	ASN	4.9
1	F	97	LEU	4.9
1	F	159	GLY	4.9
1	E	176	GLY	4.8
1	H	176	GLY	4.8
1	D	61	GLU	4.8
1	C	108	LYS	4.7
1	F	5	THR	4.7
1	J	27	GLU	4.7
1	H	7	GLN	4.7
1	B	160	LEU	4.7
1	L	167	GLU	4.7
1	H	161	MET	4.7
1	I	97	LEU	4.7
1	E	63	ARG	4.6
1	E	102	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	90	CYS	4.5
1	F	27	GLU	4.5
1	I	91	ASP	4.5
1	B	129	LEU	4.5
1	A	54	TYR	4.5
1	B	27	GLU	4.5
1	I	61	GLU	4.5
1	K	20	ILE	4.4
1	H	78	GLY	4.4
1	I	162	VAL	4.4
1	F	134	GLU	4.4
1	F	148	LEU	4.3
1	J	71	LYS	4.3
1	A	17	GLU	4.3
1	K	161	MET	4.3
1	C	17	GLU	4.3
1	B	134	GLU	4.3
1	I	27	GLU	4.3
1	I	74	ASN	4.2
1	E	164	GLY	4.2
1	I	128	HIS	4.2
1	I	160	LEU	4.2
1	J	121	ALA	4.2
1	C	27	GLU	4.2
1	H	158	MET	4.2
1	L	160	LEU	4.2
1	G	176	GLY	4.2
1	L	49	LYS	4.1
1	E	126	ASP	4.1
1	J	123	ASP	4.1
1	C	162	VAL	4.1
1	I	144	ALA	4.1
1	F	160	LEU	4.0
1	G	22	ARG	4.0
1	L	176	GLY	4.0
1	B	107	GLU	4.0
1	E	90	CYS	4.0
1	A	164	GLY	4.0
1	H	103	ALA	3.9
1	K	131	ASP	3.9
1	J	137	TYR	3.9
1	A	160	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASN	3.9
1	H	75	GLN	3.9
1	E	162	VAL	3.9
1	L	163	GLY	3.9
1	B	94	GLU	3.9
1	I	79	ARG	3.9
1	I	172	LYS	3.8
1	K	90	CYS	3.8
1	K	54	TYR	3.8
1	G	82	LEU	3.8
1	G	151	HIS	3.8
1	D	157	LYS	3.8
1	J	157	LYS	3.8
1	L	62	GLU	3.8
1	E	169	LEU	3.8
1	I	72	LEU	3.8
1	A	161	MET	3.8
1	A	71	LYS	3.8
1	D	132	PHE	3.8
1	L	151	HIS	3.7
1	J	62	GLU	3.7
1	B	30	ALA	3.7
1	L	161	MET	3.7
1	J	167	GLU	3.7
1	D	160	LEU	3.7
1	B	92	ASP	3.7
1	E	161	MET	3.7
1	E	167	GLU	3.7
1	H	61	GLU	3.7
1	G	94	GLU	3.7
1	E	48	LEU	3.6
1	K	165	LEU	3.6
1	G	161	MET	3.6
1	L	121	ALA	3.6
1	C	15	ASP	3.6
1	K	147	GLU	3.6
1	G	162	VAL	3.6
1	G	112	GLN	3.6
1	D	139	ASN	3.6
1	H	5	THR	3.6
1	B	162	VAL	3.6
1	A	139	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	107	GLU	3.6
1	I	126	ASP	3.5
1	L	123	ASP	3.5
1	J	102	CYS	3.5
1	F	164	GLY	3.5
1	L	22	ARG	3.5
1	B	163	GLY	3.5
1	D	101	GLU	3.5
1	F	123	ASP	3.5
1	B	112	GLN	3.4
1	G	72	LEU	3.4
1	L	165	LEU	3.4
1	H	17	GLU	3.4
1	I	17	GLU	3.4
1	H	92	ASP	3.4
1	K	7	GLN	3.4
1	K	158	MET	3.4
1	D	107	GLU	3.4
1	L	107	GLU	3.4
1	B	133	ILE	3.4
1	E	125	ASN	3.4
1	G	21	ASN	3.4
1	A	162	VAL	3.4
1	D	35	LEU	3.4
1	D	129	LEU	3.4
1	E	67	GLU	3.4
1	F	67	GLU	3.4
1	J	147	GLU	3.4
1	L	158	MET	3.4
1	F	147	GLU	3.4
1	J	39	TYR	3.4
1	D	165	LEU	3.3
1	I	164	GLY	3.3
1	G	79	ARG	3.3
1	I	67	GLU	3.3
1	B	95	SER	3.3
1	J	22	ARG	3.3
1	I	161	MET	3.3
1	L	102	CYS	3.3
1	K	91	ASP	3.3
1	K	159	GLY	3.3
1	F	143	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	22	ARG	3.3
1	C	16	SER	3.3
1	B	167	GLU	3.3
1	E	165	LEU	3.3
1	D	63	ARG	3.3
1	J	63	ARG	3.3
1	I	7	GLN	3.3
1	G	140	GLU	3.2
1	H	148	LEU	3.2
1	E	123	ASP	3.2
1	G	42	ASP	3.2
1	F	120	LEU	3.2
1	H	15	ASP	3.2
1	J	49	LYS	3.2
1	F	163	GLY	3.2
1	K	17	GLU	3.2
1	L	94	GLU	3.2
1	G	35	LEU	3.2
1	I	71	LYS	3.2
1	F	176	GLY	3.2
1	D	153	THR	3.2
1	I	116	GLU	3.2
1	H	81	PHE	3.1
1	G	158	MET	3.1
1	G	147	GLU	3.1
1	I	5	THR	3.1
1	H	89	ASP	3.1
1	I	60	HIS	3.1
1	J	134	GLU	3.1
1	A	175	LEU	3.1
1	H	123	ASP	3.1
1	C	155	LEU	3.1
1	J	103	ALA	3.1
1	B	161	MET	3.1
1	E	150	ASP	3.1
1	I	176	GLY	3.1
1	J	163	GLY	3.1
1	C	107	GLU	3.1
1	D	27	GLU	3.1
1	D	161	MET	3.0
1	A	95	SER	3.0
1	K	75	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	61	GLU	3.0
1	D	6	SER	3.0
1	H	113	SER	3.0
1	I	150	ASP	3.0
1	A	14	GLN	3.0
1	C	101	GLU	3.0
1	C	8	VAL	3.0
1	G	46	VAL	3.0
1	J	161	MET	3.0
1	L	157	LYS	3.0
1	F	125	ASN	3.0
1	L	58	GLN	3.0
1	E	62	GLU	3.0
1	E	121	ALA	3.0
1	B	142	VAL	3.0
1	A	7	GLN	3.0
1	J	129	LEU	3.0
1	A	118	HIS	3.0
1	E	40	TYR	2.9
1	E	86	GLN	2.9
1	B	120	LEU	2.9
1	G	48	LEU	2.9
1	C	83	GLN	2.9
1	B	64	GLU	2.9
1	D	167	GLU	2.9
1	G	67	GLU	2.9
1	K	128	HIS	2.9
1	C	115	LEU	2.9
1	K	176	GLY	2.9
1	A	134	GLU	2.9
1	B	150	ASP	2.9
1	I	125	ASN	2.9
1	A	65	HIS	2.9
1	K	13	HIS	2.9
1	H	85	ILE	2.9
1	J	160	LEU	2.9
1	H	159	GLY	2.9
1	I	159	GLY	2.9
1	H	94	GLU	2.9
1	L	71	LYS	2.9
1	G	174	THR	2.9
1	I	20	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	102	CYS	2.9
1	E	112	GLN	2.8
1	D	137	TYR	2.8
1	H	67	GLU	2.8
1	I	63	ARG	2.8
1	J	60	HIS	2.8
1	K	35	LEU	2.8
1	C	161	MET	2.8
1	C	14	GLN	2.8
1	I	143	LYS	2.8
1	G	116	GLU	2.8
1	L	19	ALA	2.8
1	L	42	ASP	2.8
1	J	176	GLY	2.8
1	A	27	GLU	2.8
1	F	151	HIS	2.8
1	L	148	LEU	2.8
1	E	163	GLY	2.8
1	K	164	GLY	2.8
1	C	141	GLN	2.8
1	F	75	GLN	2.8
1	K	61	GLU	2.8
1	K	64	GLU	2.8
1	B	132	PHE	2.8
1	C	80	ILE	2.8
1	I	35	LEU	2.8
1	L	139	ASN	2.8
1	E	49	LYS	2.8
1	B	17	GLU	2.7
1	K	62	GLU	2.7
1	K	79	ARG	2.7
1	D	166	ALA	2.7
1	I	68	LYS	2.7
1	K	68	LYS	2.7
1	H	91	ASP	2.7
1	I	131	ASP	2.7
1	D	163	GLY	2.7
1	J	164	GLY	2.7
1	E	66	ALA	2.7
1	L	82	LEU	2.7
1	K	151	HIS	2.7
1	B	62	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	94	GLU	2.7
1	G	160	LEU	2.7
1	I	120	LEU	2.7
1	G	49	LYS	2.7
1	H	102	CYS	2.7
1	I	151	HIS	2.7
1	F	42	ASP	2.7
1	E	142	VAL	2.7
1	I	33	VAL	2.7
1	H	110	VAL	2.7
1	K	94	GLU	2.7
1	A	155	LEU	2.7
1	C	113	SER	2.7
1	F	81	PHE	2.6
1	D	158	MET	2.6
1	J	100	MET	2.6
1	D	75	GLN	2.6
1	H	62	GLU	2.6
1	A	60	HIS	2.6
1	G	60	HIS	2.6
1	C	166	ALA	2.6
1	B	117	LEU	2.6
1	G	169	LEU	2.6
1	B	7	GLN	2.6
1	F	107	GLU	2.6
1	J	66	ALA	2.6
1	K	15	ASP	2.6
1	L	103	ALA	2.6
1	G	65	HIS	2.6
1	G	113	SER	2.6
1	J	53	LYS	2.6
1	L	53	LYS	2.6
1	H	163	GLY	2.6
1	L	147	GLU	2.6
1	I	132	PHE	2.6
1	L	154	ASN	2.6
1	L	159	GLY	2.5
1	L	164	GLY	2.5
1	E	168	TYR	2.5
1	A	62	GLU	2.5
1	C	7	GLN	2.5
1	G	167	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	64	GLU	2.5
1	L	112	GLN	2.5
1	D	150	ASP	2.5
1	G	126	ASP	2.5
1	J	151	HIS	2.5
1	B	157	LYS	2.5
1	J	96	GLY	2.5
1	L	129	LEU	2.5
1	L	138	LEU	2.5
1	E	39	TYR	2.5
1	C	134	GLU	2.5
1	E	174	THR	2.5
1	F	86	GLN	2.5
1	H	83	GLN	2.5
1	L	7	GLN	2.5
1	H	65	HIS	2.5
1	D	123	ASP	2.5
1	E	91	ASP	2.5
1	K	78	GLY	2.5
1	G	142	VAL	2.5
1	J	8	VAL	2.5
1	A	94	GLU	2.5
1	B	14	GLN	2.5
1	B	125	ASN	2.5
1	C	74	ASN	2.5
1	I	123	ASP	2.5
1	J	38	SER	2.5
1	K	36	SER	2.5
1	C	110	VAL	2.5
1	L	101	GLU	2.5
1	L	63	ARG	2.5
1	F	135	THR	2.5
1	L	99	ALA	2.5
1	L	172	LYS	2.5
1	B	65	HIS	2.5
1	E	128	HIS	2.5
1	F	173	HIS	2.5
1	C	90	CYS	2.5
1	L	109	ASN	2.5
1	D	148	LEU	2.4
1	C	159	GLY	2.4
1	B	101	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	79	ARG	2.4
1	E	140	GLU	2.4
1	G	62	GLU	2.4
1	L	116	GLU	2.4
1	L	134	GLU	2.4
1	L	140	GLU	2.4
1	F	121	ALA	2.4
1	I	141	GLN	2.4
1	E	160	LEU	2.4
1	F	35	LEU	2.4
1	F	114	LEU	2.4
1	A	24	ILE	2.4
1	A	8	VAL	2.4
1	B	124	LYS	2.4
1	B	137	TYR	2.4
1	I	165	LEU	2.4
1	C	89	ASP	2.4
1	K	33	VAL	2.4
1	B	53	LYS	2.4
1	J	119	LYS	2.4
1	K	143	LYS	2.4
1	A	132	PHE	2.4
1	H	153	THR	2.4
1	G	105	HIS	2.4
1	H	97	LEU	2.4
1	F	63	ARG	2.4
1	K	123	ASP	2.4
1	G	144	ALA	2.4
1	C	137	TYR	2.4
1	F	158	MET	2.4
1	G	153	THR	2.4
1	K	100	MET	2.4
1	E	33	VAL	2.3
1	C	123	ASP	2.3
1	D	15	ASP	2.3
1	G	19	ALA	2.3
1	F	161	MET	2.3
1	C	13	HIS	2.3
1	E	20	ILE	2.3
1	C	157	LYS	2.3
1	F	68	LYS	2.3
1	G	139	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	132	PHE	2.3
1	D	42	ASP	2.3
1	H	167	GLU	2.3
1	A	58	GLN	2.3
1	C	138	LEU	2.3
1	D	16	SER	2.3
1	B	153	THR	2.3
1	G	53	LYS	2.3
1	G	63	ARG	2.3
1	D	162	VAL	2.3
1	H	149	GLY	2.3
1	C	125	ASN	2.3
1	F	144	ALA	2.3
1	B	123	ASP	2.3
1	B	126	ASP	2.3
1	I	148	LEU	2.3
1	J	69	LEU	2.3
1	F	113	SER	2.3
1	G	71	LYS	2.3
1	J	128	HIS	2.3
1	K	5	THR	2.3
1	L	174	THR	2.3
1	L	142	VAL	2.3
1	G	81	PHE	2.3
1	G	98	ASN	2.3
1	I	81	PHE	2.3
1	E	18	ALA	2.3
1	G	61	GLU	2.3
1	K	103	ALA	2.3
1	A	117	LEU	2.3
1	B	141	GLN	2.3
1	I	138	LEU	2.3
1	L	79	ARG	2.3
1	A	137	TYR	2.3
1	H	137	TYR	2.3
1	J	40	TYR	2.3
1	F	8	VAL	2.3
1	F	166	ALA	2.2
1	G	155	LEU	2.2
1	D	49	LYS	2.2
1	D	92	ASP	2.2
1	E	89	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	174	THR	2.2
1	B	54	TYR	2.2
1	C	81	PHE	2.2
1	B	67	GLU	2.2
1	E	28	LEU	2.2
1	E	45	ASP	2.2
1	E	136	HIS	2.2
1	G	90	CYS	2.2
1	J	33	VAL	2.2
1	A	59	SER	2.2
1	J	31	SER	2.2
1	G	170	PHE	2.2
1	A	148	LEU	2.2
1	E	26	LEU	2.2
1	G	99	ALA	2.2
1	L	133	ILE	2.2
1	D	90	CYS	2.2
1	B	96	GLY	2.2
1	H	114	LEU	2.2
1	H	160	LEU	2.2
1	G	47	ALA	2.2
1	L	67	GLU	2.2
1	G	14	GLN	2.2
1	J	74	ASN	2.2
1	L	136	HIS	2.2
1	B	152	VAL	2.2
1	F	131	ASP	2.2
1	H	126	ASP	2.2
1	J	131	ASP	2.2
1	E	100	MET	2.2
1	I	49	LYS	2.2
1	K	137	TYR	2.2
1	D	72	LEU	2.2
1	H	106	LEU	2.2
1	E	166	ALA	2.2
1	G	121	ALA	2.2
1	B	80	ILE	2.1
1	K	42	ASP	2.1
1	L	171	ASP	2.1
1	A	163	GLY	2.1
1	J	149	GLY	2.1
1	E	55	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	165	LEU	2.1
1	C	38	SER	2.1
1	F	90	CYS	2.1
1	H	99	ALA	2.1
1	A	9	ARG	2.1
1	F	76	ARG	2.1
1	G	145	ILE	2.1
1	D	125	ASN	2.1
1	B	46	VAL	2.1
1	D	110	VAL	2.1
1	F	162	VAL	2.1
1	J	44	ASP	2.1
1	D	81	PHE	2.1
1	E	35	LEU	2.1
1	D	62	GLU	2.1
1	K	167	GLU	2.1
1	D	14	GLN	2.1
1	F	14	GLN	2.1
1	I	73	GLN	2.1
1	L	86	GLN	2.1
1	E	143	LYS	2.1
1	G	37	MET	2.1
1	L	111	ASN	2.1
1	C	150	ASP	2.1
1	D	149	GLY	2.1
1	E	159	GLY	2.1
1	J	126	ASP	2.1
1	A	140	GLU	2.1
1	A	167	GLU	2.1
1	D	168	TYR	2.1
1	B	31	SER	2.1
1	E	59	SER	2.1
1	E	73	GLN	2.1
1	C	60	HIS	2.1
1	K	124	LYS	2.1
1	A	125	ASN	2.1
1	J	109	ASN	2.1
1	C	106	LEU	2.1
1	G	166	ALA	2.1
1	I	62	GLU	2.1
1	I	147	GLU	2.1
1	B	39	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	143	LYS	2.0
1	J	142	VAL	2.0
1	J	139	ASN	2.0
1	J	174	THR	2.0
1	D	126	ASP	2.0
1	A	61	GLU	2.0
1	A	101	GLU	2.0
1	B	93	TRP	2.0
1	D	116	GLU	2.0
1	F	62	GLU	2.0
1	D	37	MET	2.0
1	F	128	HIS	2.0
1	A	56	LEU	2.0
1	H	129	LEU	2.0
1	A	81	PHE	2.0
1	C	164	GLY	2.0
1	L	122	THR	2.0
1	G	91	ASP	2.0
1	L	92	ASP	2.0
1	B	119	LYS	2.0
1	D	68	LYS	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.