Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:33 PM GMT

PDB ID	:	3RE7
Title	:	Copper (II) loaded Bullfrog Ferritin M chain
Authors	:	Bertini, I.; Lalli, D.; Mangani, S.; Pozzi, C.; Rosa, C.; Turano, P.
Deposited on	:	2011-04-02
Resolution	:	2.82 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

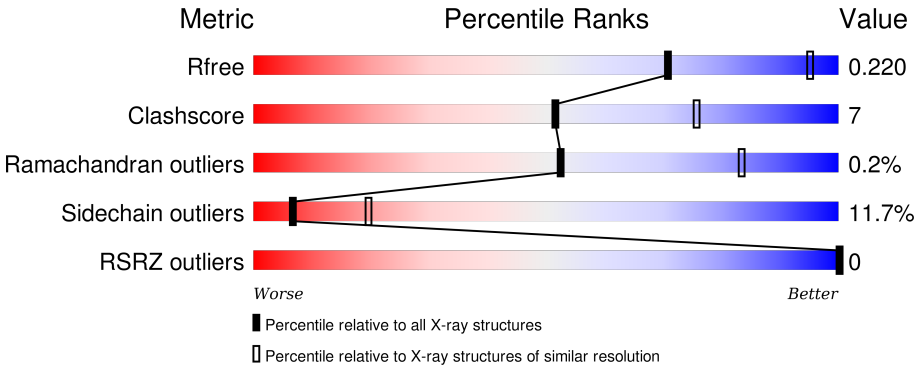
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	176	77% 16%
1	B	176	75% 19%
1	C	176	73% 21%
1	D	176	76% 19%
1	E	176	72% 22%

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Mol	Chain	Length	Quality of chain
1	F	176	73% 22%
1	G	176	76% 18%
1	H	176	77% 18%
1	I	176	75% 19%
1	J	176	74% 19%
1	K	176	72% 22% 5%
1	L	176	74% 19%
1	M	176	75% 19%
1	N	176	76% 19%
1	O	176	76% 18%
1	P	176	75% 20%
1	Q	176	70% 26%
1	R	176	78% 15% 5%
1	S	176	71% 22% 5%
1	T	176	76% 19%
1	U	176	71% 23%
1	V	176	74% 18% 5%
1	W	176	71% 23%
1	X	176	73% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	D	191	-	-	X	-
2	CU	H	177	-	-	-	X
2	CU	M	182	-	-	-	X
2	CU	P	181	-	-	-	X
2	CU	R	192	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	T	181	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34999 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, middle subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	B	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	C	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	D	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	E	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	F	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	G	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	H	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	I	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	J	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	K	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	L	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	M	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	N	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	O	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	P	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	R	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	S	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	T	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	U	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	V	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	W	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	X	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	6	Total	Cu	0	0
			6	6		
2	K	6	Total	Cu	0	0
			6	6		
2	B	8	Total	Cu	0	0
			8	8		
2	W	6	Total	Cu	0	0
			6	6		
2	N	7	Total	Cu	0	0
			7	7		
2	X	6	Total	Cu	0	0
			6	6		
2	S	5	Total	Cu	0	0
			5	5		
2	J	8	Total	Cu	0	0
			8	8		
2	E	8	Total	Cu	0	0
			8	8		
2	V	5	Total	Cu	0	0
			5	5		
2	A	8	Total	Cu	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	7	Total Cu 7 7	0	0
2	M	8	Total Cu 8 8	0	0
2	D	10	Total Cu 10 10	0	0
2	I	7	Total Cu 7 7	0	0
2	U	6	Total Cu 6 6	0	0
2	L	7	Total Cu 7 7	0	0
2	G	8	Total Cu 8 8	0	0
2	Q	6	Total Cu 6 6	0	0
2	H	7	Total Cu 7 7	0	0
2	C	7	Total Cu 7 7	0	0
2	T	4	Total Cu 4 4	0	0
2	O	6	Total Cu 6 6	0	0
2	F	6	Total Cu 6 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	42	Total O 42 42	0	0
3	B	22	Total O 22 22	0	0
3	C	34	Total O 34 34	0	0
3	D	31	Total O 31 31	0	0
3	E	22	Total O 22 22	0	0
3	F	28	Total O 28 28	0	0

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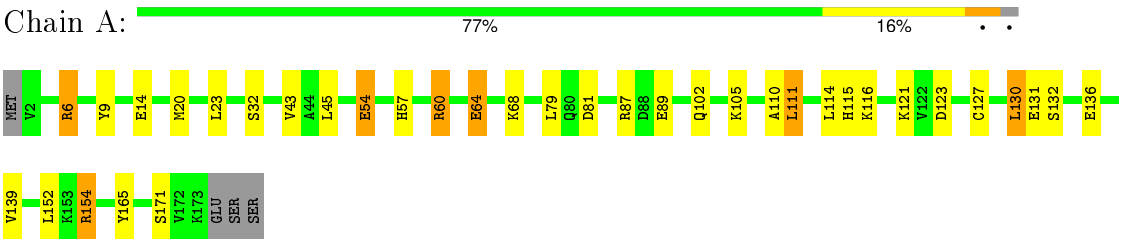
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	31	Total O 31 31	0	0
3	H	35	Total O 35 35	0	0
3	I	24	Total O 24 24	0	0
3	J	44	Total O 44 44	0	0
3	K	48	Total O 48 48	0	0
3	L	19	Total O 19 19	0	0
3	M	30	Total O 30 30	0	0
3	N	41	Total O 41 41	0	0
3	O	31	Total O 31 31	0	0
3	P	32	Total O 32 32	0	0
3	Q	41	Total O 41 41	0	0
3	R	41	Total O 41 41	0	0
3	S	35	Total O 35 35	0	0
3	T	29	Total O 29 29	0	0
3	U	41	Total O 41 41	0	0
3	V	20	Total O 20 20	0	0
3	W	41	Total O 41 41	0	0
3	X	43	Total O 43 43	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

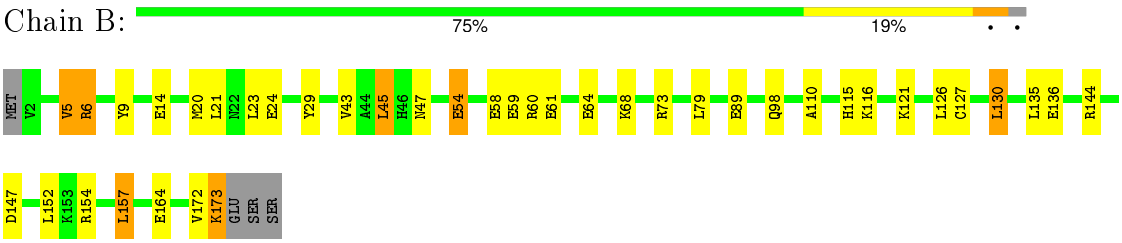
- Molecule 1: Ferritin, middle subunit

Chain A:



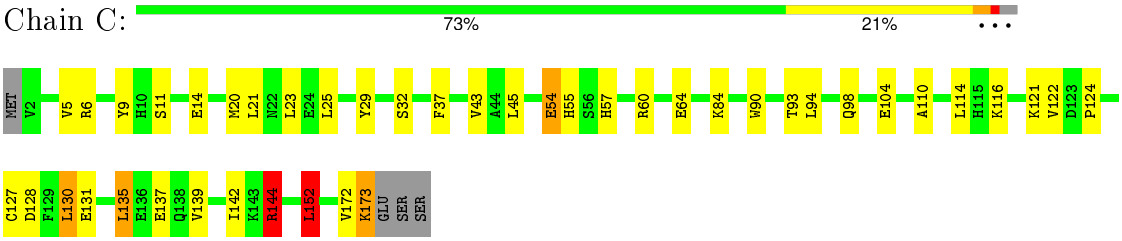
- Molecule 1: Ferritin, middle subunit

Chain B:



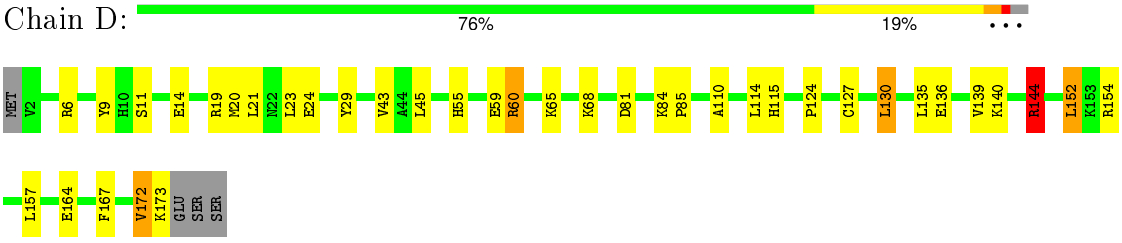
- Molecule 1: Ferritin, middle subunit

Chain C:



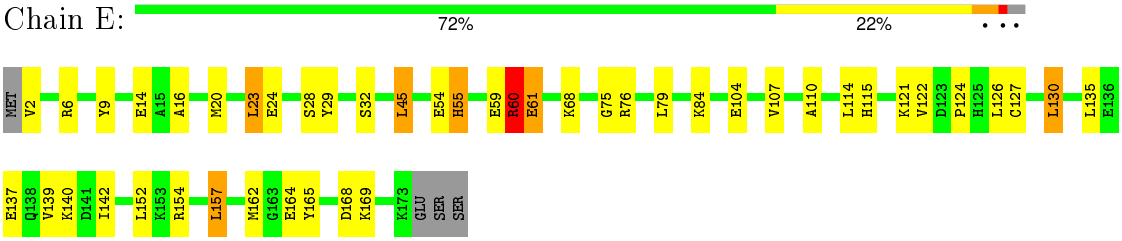
- Molecule 1: Ferritin, middle subunit

Chain D:



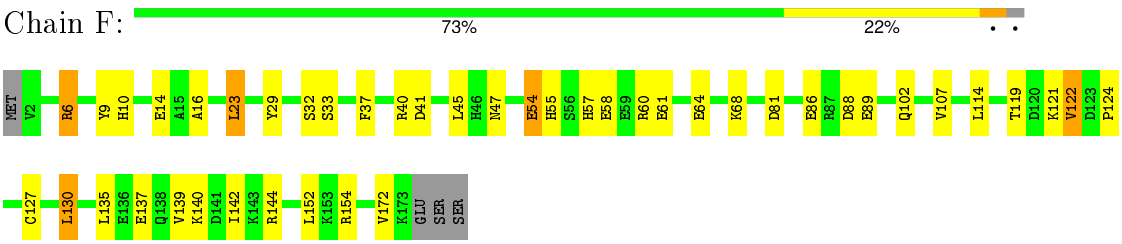
• Molecule 1: Ferritin, middle subunit

Chain E:



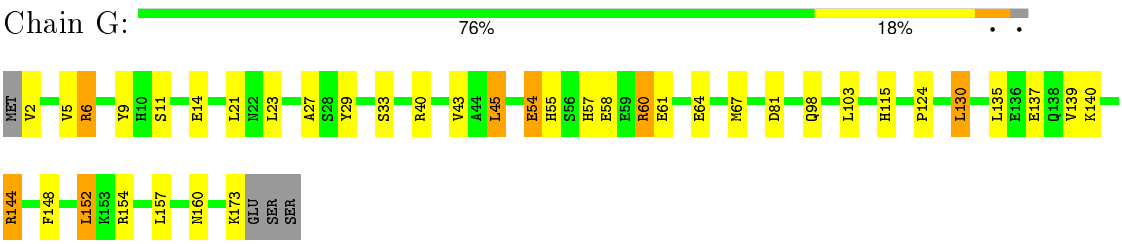
• Molecule 1: Ferritin, middle subunit

Chain F:



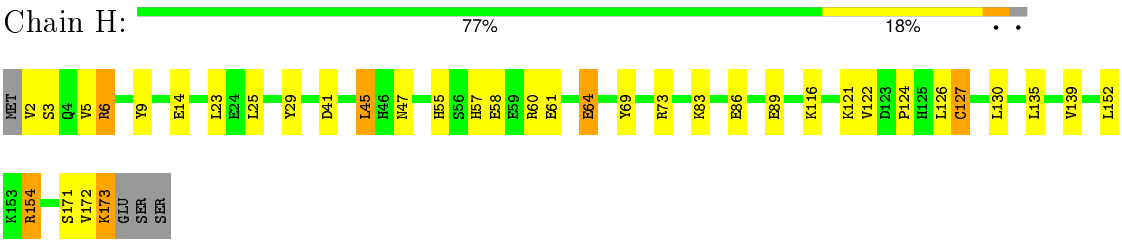
• Molecule 1: Ferritin, middle subunit

Chain G:



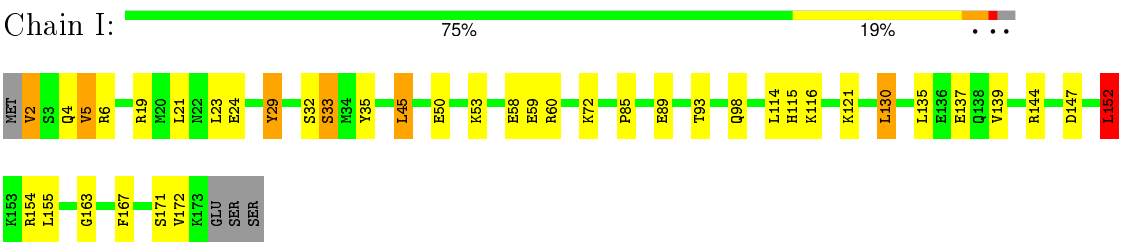
• Molecule 1: Ferritin, middle subunit

Chain H:



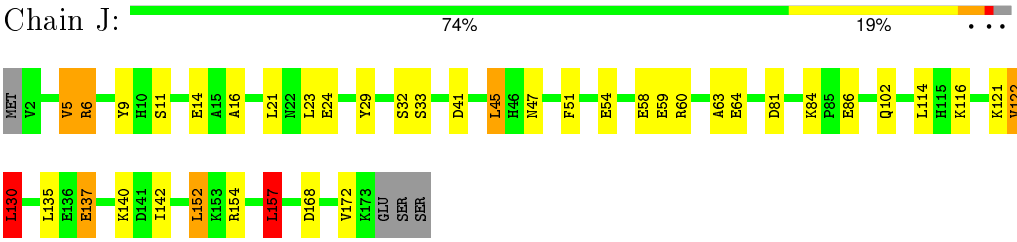
• Molecule 1: Ferritin, middle subunit

Chain I:



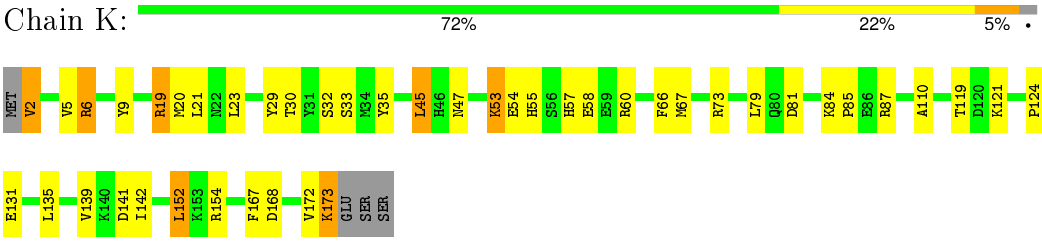
• Molecule 1: Ferritin, middle subunit

Chain J:



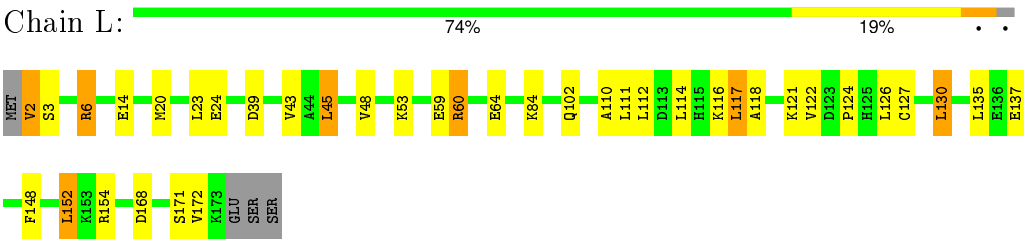
- Molecule 1: Ferritin, middle subunit

Chain K:



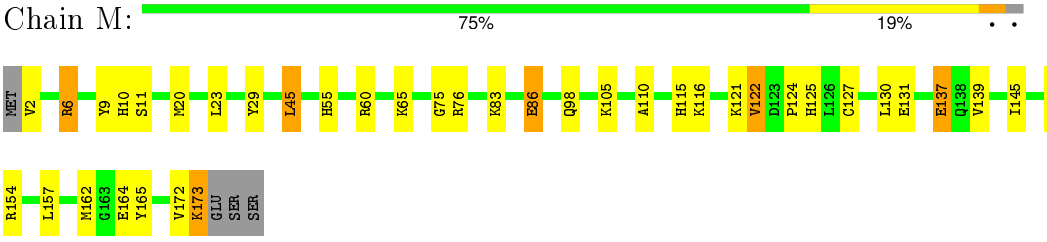
- Molecule 1: Ferritin, middle subunit

Chain L:



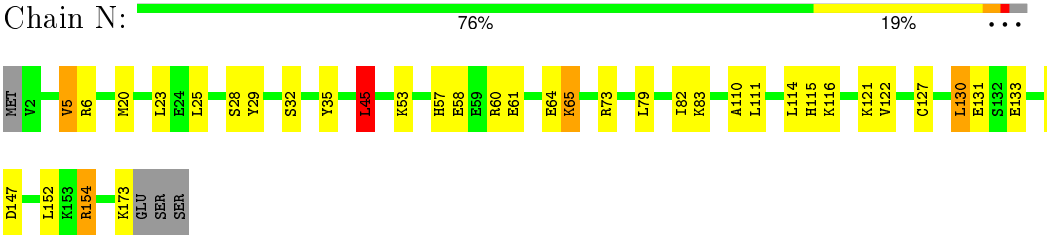
- Molecule 1: Ferritin, middle subunit

Chain M:



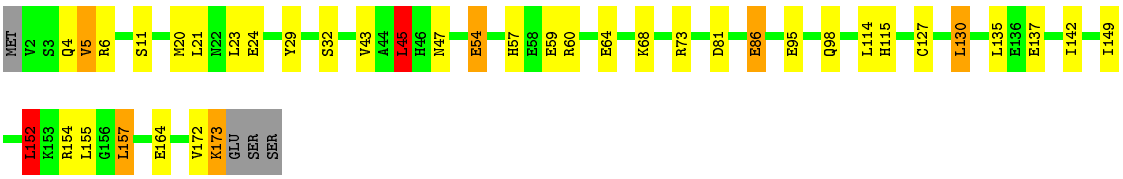
- Molecule 1: Ferritin, middle subunit

Chain N:



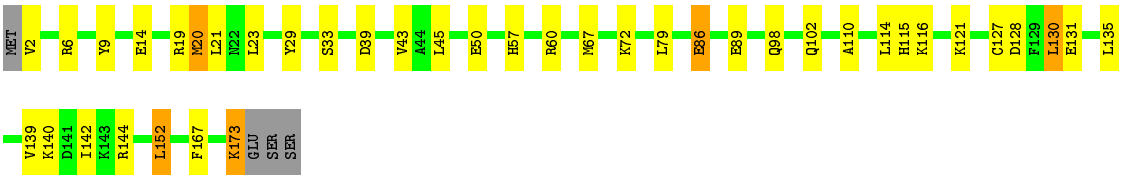
- Molecule 1: Ferritin, middle subunit

Chain O:



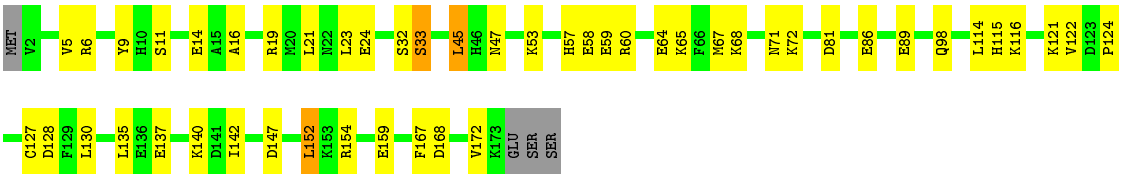
• Molecule 1: Ferritin, middle subunit

Chain P:



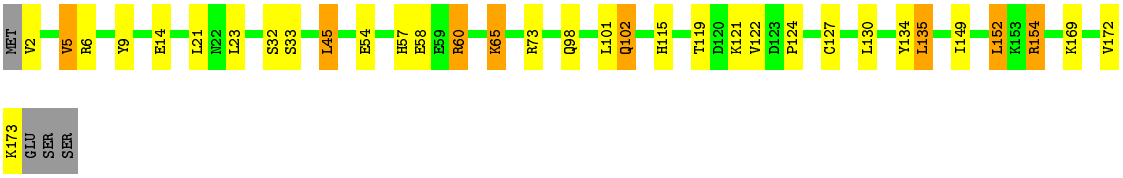
• Molecule 1: Ferritin, middle subunit

Chain Q:



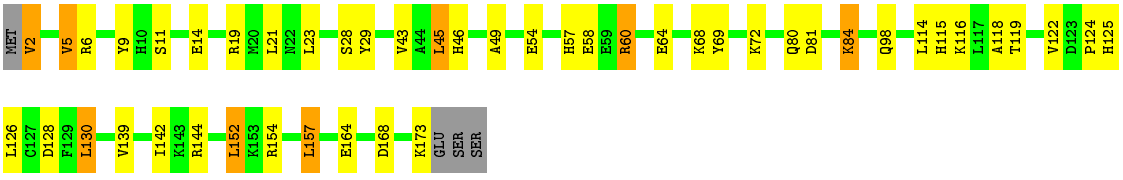
• Molecule 1: Ferritin, middle subunit

Chain R:



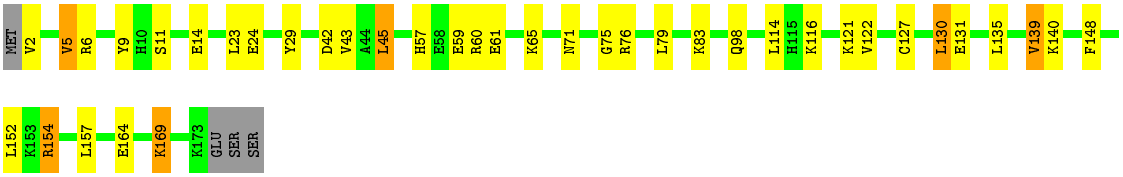
• Molecule 1: Ferritin, middle subunit

Chain S:



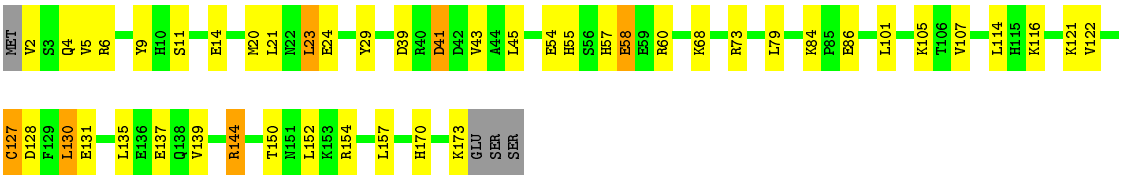
• Molecule 1: Ferritin, middle subunit

Chain T:



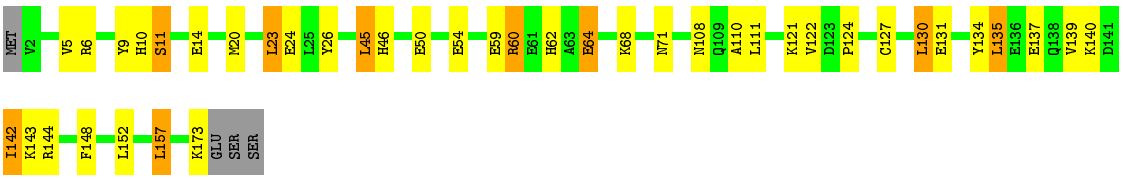
• Molecule 1: Ferritin, middle subunit

Chain U:



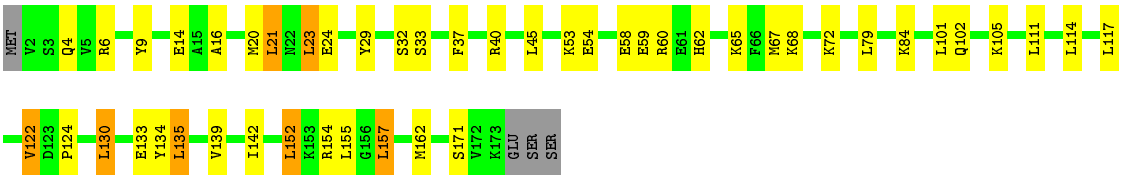
• Molecule 1: Ferritin, middle subunit

Chain V:



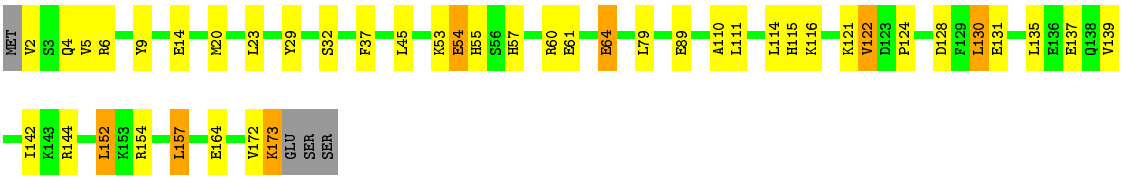
• Molecule 1: Ferritin, middle subunit

Chain W:



• Molecule 1: Ferritin, middle subunit

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.21Å 210.21Å 322.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 2.82 48.19 – 2.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.50-2.82) 99.9 (48.19-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.170 , 0.224 0.170 , 0.220	Depositor DCC
R_{free} test set	9961 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 28.1	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 197893 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	34999	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	1.06	5/1446 (0.3%)	1.00	7/1944 (0.4%)
1	B	0.99	4/1446 (0.3%)	0.91	2/1944 (0.1%)
1	C	0.98	1/1446 (0.1%)	0.93	2/1944 (0.1%)
1	D	1.01	0/1446	0.94	1/1944 (0.1%)
1	E	0.97	1/1446 (0.1%)	0.90	1/1944 (0.1%)
1	F	1.01	3/1446 (0.2%)	0.89	3/1944 (0.2%)
1	G	1.06	2/1446 (0.1%)	0.93	4/1944 (0.2%)
1	H	1.04	4/1446 (0.3%)	0.95	2/1944 (0.1%)
1	I	0.95	3/1446 (0.2%)	0.94	4/1944 (0.2%)
1	J	1.09	4/1446 (0.3%)	0.95	5/1944 (0.3%)
1	K	1.03	2/1446 (0.1%)	1.01	6/1944 (0.3%)
1	L	1.00	1/1446 (0.1%)	0.92	3/1944 (0.2%)
1	M	1.01	1/1446 (0.1%)	0.92	3/1944 (0.2%)
1	N	1.05	3/1446 (0.2%)	0.98	5/1944 (0.3%)
1	O	1.03	1/1446 (0.1%)	0.95	4/1944 (0.2%)
1	P	0.99	2/1446 (0.1%)	0.92	2/1944 (0.1%)
1	Q	1.04	2/1446 (0.1%)	0.96	6/1944 (0.3%)
1	R	1.02	3/1446 (0.2%)	0.95	3/1944 (0.2%)
1	S	1.00	4/1446 (0.3%)	0.93	3/1944 (0.2%)
1	T	0.99	3/1446 (0.2%)	0.93	0/1944
1	U	1.03	3/1446 (0.2%)	0.92	0/1944
1	V	1.00	2/1446 (0.1%)	0.90	1/1944 (0.1%)
1	W	1.02	2/1446 (0.1%)	0.93	1/1944 (0.1%)
1	X	1.09	4/1446 (0.3%)	0.93	0/1944
All	All	1.02	60/34704 (0.2%)	0.94	68/46656 (0.1%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLU	CG-CD	7.97	1.64	1.51
1	X	131	GLU	CG-CD	7.86	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLU	CG-CD	7.73	1.63	1.51
1	O	54	GLU	CG-CD	7.62	1.63	1.51
1	E	54	GLU	CG-CD	7.54	1.63	1.51
1	N	61	GLU	CG-CD	7.41	1.63	1.51
1	C	54	GLU	CG-CD	7.41	1.63	1.51
1	G	54	GLU	CG-CD	7.36	1.62	1.51
1	R	58	GLU	CG-CD	7.30	1.62	1.51
1	H	127	CYS	CB-SG	7.05	1.94	1.82
1	B	61	GLU	CB-CG	7.04	1.65	1.52
1	U	127	CYS	CB-SG	6.75	1.93	1.82
1	J	54	GLU	CG-CD	6.71	1.62	1.51
1	X	54	GLU	CG-CD	6.68	1.61	1.51
1	B	54	GLU	CG-CD	6.58	1.61	1.51
1	P	50	GLU	CG-CD	6.35	1.61	1.51
1	Q	58	GLU	CG-CD	6.30	1.61	1.51
1	H	61	GLU	CG-CD	6.29	1.61	1.51
1	M	137	GLU	CG-CD	6.24	1.61	1.51
1	K	141	ASP	CB-CG	6.23	1.64	1.51
1	R	54	GLU	CG-CD	6.21	1.61	1.51
1	G	58	GLU	CG-CD	6.18	1.61	1.51
1	F	64	GLU	CG-CD	6.14	1.61	1.51
1	U	58	GLU	CG-CD	6.02	1.60	1.51
1	X	64	GLU	CG-CD	6.02	1.60	1.51
1	N	61	GLU	CB-CG	5.91	1.63	1.52
1	V	54	GLU	CG-CD	5.90	1.60	1.51
1	L	64	GLU	CG-CD	5.89	1.60	1.51
1	U	54	GLU	CG-CD	5.89	1.60	1.51
1	W	58	GLU	CG-CD	5.87	1.60	1.51
1	A	60	ARG	CG-CD	5.86	1.66	1.51
1	S	54	GLU	CG-CD	5.81	1.60	1.51
1	R	102	GLN	CG-CD	5.71	1.64	1.51
1	K	54	GLU	CG-CD	5.68	1.60	1.51
1	T	2	VAL	CB-CG2	5.68	1.64	1.52
1	I	58	GLU	CG-CD	5.66	1.60	1.51
1	J	137	GLU	CG-CD	5.57	1.60	1.51
1	H	58	GLU	CG-CD	5.55	1.60	1.51
1	F	54	GLU	CG-CD	5.54	1.60	1.51
1	A	64	GLU	CG-CD	5.51	1.60	1.51
1	H	64	GLU	CG-CD	5.44	1.60	1.51
1	T	61	GLU	CB-CG	5.41	1.62	1.52
1	P	86	GLU	CG-CD	5.41	1.60	1.51
1	B	58	GLU	CG-CD	5.40	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	58	GLU	CG-CD	5.38	1.60	1.51
1	J	58	GLU	CG-CD	5.33	1.59	1.51
1	W	54	GLU	CG-CD	5.33	1.59	1.51
1	S	2	VAL	CB-CG2	5.26	1.63	1.52
1	X	131	GLU	CB-CG	5.24	1.62	1.52
1	A	102	GLN	CG-CD	5.21	1.63	1.51
1	T	61	GLU	CG-CD	5.17	1.59	1.51
1	J	64	GLU	CG-CD	5.16	1.59	1.51
1	I	2	VAL	CB-CG2	5.16	1.63	1.52
1	N	58	GLU	CG-CD	5.13	1.59	1.51
1	A	136	GLU	CB-CG	5.05	1.61	1.52
1	S	58	GLU	CG-CD	5.05	1.59	1.51
1	I	50	GLU	CG-CD	5.04	1.59	1.51
1	V	64	GLU	CG-CD	5.03	1.59	1.51
1	Q	159	GLU	CG-CD	5.02	1.59	1.51
1	S	64	GLU	CB-CG	5.00	1.61	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	6	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	N	6	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	I	6	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	K	19	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	6	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	J	6	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	M	6	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	144	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	R	60	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	G	6	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	81	ASP	CB-CG-OD1	6.97	124.57	118.30
1	S	19	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	G	40	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	H	154	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	J	6	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	K	19	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	M	6	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	87	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	R	152	LEU	CA-CB-CG	6.25	129.68	115.30
1	K	87	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	B	6	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	Q	154	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	72	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	R	154	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	I	19	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	J	81	ASP	CB-CG-OD1	5.90	123.61	118.30
1	N	154	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	6	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	O	21	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	N	154	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	154	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	S	81	ASP	CB-CG-OD1	5.79	123.52	118.30
1	B	45	LEU	CA-CB-CG	5.76	128.54	115.30
1	K	2	VAL	CB-CA-C	-5.76	100.46	111.40
1	P	20	MET	CG-SD-CE	-5.75	91.00	100.20
1	S	81	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	144	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	H	154	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	W	21	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	F	6	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	Q	147	ASP	CB-CG-OD1	5.56	123.30	118.30
1	Q	81	ASP	CB-CG-OD1	5.50	123.25	118.30
1	L	6	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	L	117	LEU	CA-CB-CG	5.39	127.69	115.30
1	L	45	LEU	CA-CB-CG	5.38	127.67	115.30
1	E	60	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	V	130	LEU	CA-CB-CG	5.28	127.45	115.30
1	J	130	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	81	ASP	CB-CG-OD1	5.24	123.02	118.30
1	K	6	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	I	72	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	O	6	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	81	ASP	CB-CG-OD1	5.17	122.95	118.30
1	K	81	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	111	LEU	CA-CB-CG	5.16	127.18	115.30
1	O	45	LEU	CA-CB-CG	5.16	127.16	115.30
1	M	45	LEU	CA-CB-CG	5.14	127.13	115.30
1	C	152	LEU	CA-CB-CG	5.13	127.10	115.30
1	G	45	LEU	CB-CG-CD1	5.12	119.70	111.00
1	O	152	LEU	CA-CB-CG	5.09	127.00	115.30
1	F	88	ASP	CB-CG-OD1	5.09	122.88	118.30
1	N	45	LEU	CA-CB-CG	5.08	126.98	115.30
1	I	152	LEU	CA-CB-CG	5.07	126.97	115.30
1	P	144	ARG	NE-CZ-NH1	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	81	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	A	60	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	Q	19	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	J	157	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1418	0	1369	23	0
1	B	1418	0	1369	24	0
1	C	1418	0	1369	26	0
1	D	1418	0	1370	23	0
1	E	1418	0	1369	28	0
1	F	1418	0	1369	20	0
1	G	1418	0	1369	27	0
1	H	1418	0	1369	19	0
1	I	1418	0	1369	22	0
1	J	1418	0	1369	19	0
1	K	1418	0	1369	32	0
1	L	1418	0	1369	22	0
1	M	1418	0	1369	25	0
1	N	1418	0	1369	19	0
1	O	1418	0	1369	25	0
1	P	1418	0	1369	23	0
1	Q	1418	0	1369	20	0
1	R	1418	0	1369	20	0
1	S	1418	0	1369	30	0
1	T	1418	0	1369	24	0
1	U	1418	0	1369	25	0
1	V	1418	0	1369	26	0
1	W	1418	0	1369	36	0
1	X	1418	0	1370	25	0
2	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	0	0	0
2	C	7	0	0	0	0
2	D	10	0	0	3	0
2	E	8	0	0	0	0
2	F	6	0	0	0	0
2	G	8	0	0	0	0
2	H	7	0	0	0	0
2	I	7	0	0	0	0
2	J	8	0	0	0	0
2	K	6	0	0	0	0
2	L	7	0	0	0	0
2	M	8	0	0	0	0
2	N	7	0	0	0	0
2	O	6	0	0	0	0
2	P	6	0	0	0	0
2	Q	6	0	0	0	0
2	R	7	0	0	0	0
2	S	5	0	0	0	0
2	T	4	0	0	0	0
2	U	6	0	0	0	0
2	V	5	0	0	0	0
2	W	6	0	0	0	0
2	X	6	0	0	0	0
3	A	42	0	0	3	0
3	B	22	0	0	1	0
3	C	34	0	0	1	0
3	D	31	0	0	5	0
3	E	22	0	0	2	0
3	F	28	0	0	2	0
3	G	31	0	0	1	0
3	H	35	0	0	3	0
3	I	24	0	0	3	0
3	J	44	0	0	1	0
3	K	48	0	0	0	0
3	L	19	0	0	1	0
3	M	30	0	0	2	0
3	N	41	0	0	3	0
3	O	31	0	0	5	0
3	P	32	0	0	2	0
3	Q	41	0	0	3	0
3	R	41	0	0	0	0
3	S	35	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	29	0	0	1	0
3	U	41	0	0	3	0
3	V	20	0	0	2	0
3	W	41	0	0	6	0
3	X	43	0	0	1	0
All	All	34999	0	32858	453	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 7.

All (453) 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:D:144:ARG:HD2	3:D:663:HOH:O	1.52	1.09
1:I:144:ARG:HD2	3:I:274:HOH:O	1.58	1.03
1:P:173:LYS:H	1:P:173:LYS:HD3	1.22	1.01
1:A:57:HIS:HB3	3:A:673:HOH:O	1.61	0.99
1:A:60:ARG:HD3	1:G:60:ARG:NE	1.76	0.99
1:C:60:ARG:HD3	1:O:60:ARG:HD2	1.51	0.92
1:S:118:ALA:HB2	1:S:126:LEU:HD23	1.54	0.89
1:D:127:CYS:HG	2:D:191:CU:CU	0.85	0.86
1:T:6:ARG:NH2	1:T:14:GLU:OE1	2.08	0.86
1:P:173:LYS:H	1:P:173:LYS:CD	1.87	0.86
1:V:148:PHE:O	1:V:152:LEU:HD22	1.76	0.84
1:C:142:ILE:HG22	1:S:5:VAL:HG22	1.57	0.83
1:K:60:ARG:HD3	1:W:60:ARG:HD3	1.58	0.83
1:X:6:ARG:NH1	1:X:9:TYR:O	2.13	0.82
1:C:6:ARG:NH2	1:C:14:GLU:OE1	2.13	0.81
1:W:6:ARG:NH1	1:W:9:TYR:O	2.14	0.80
1:D:84:LYS:NZ	3:D:193:HOH:O	2.10	0.80
1:P:6:ARG:NH1	1:P:9:TYR:O	2.14	0.80
1:C:131:GLU:HG2	1:S:128:ASP:HB2	1.64	0.78
1:J:142:ILE:HG22	1:N:5:VAL:HG22	1.66	0.78
1:D:154:ARG:NH2	1:K:45:LEU:HD13	2.00	0.77
1:A:60:ARG:HD3	1:G:60:ARG:HE	1.46	0.77
1:L:122:VAL:O	1:L:122:VAL:HG12	1.84	0.76
1:L:6:ARG:NH2	1:L:14:GLU:OE1	2.16	0.76
1:Q:6:ARG:NH2	1:Q:14:GLU:OE1	2.17	0.76
1:R:5:VAL:HG22	1:S:142:ILE:HG22	1.68	0.75
1:D:6:ARG:NH2	1:D:14:GLU:OE1	2.19	0.75
1:Q:6:ARG:NH1	1:Q:9:TYR:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH2	1:A:14:GLU:OE1	2.17	0.75
1:J:6:ARG:NH1	1:J:9:TYR:O	2.19	0.75
1:K:142:ILE:HG22	1:U:5:VAL:HG22	1.69	0.75
1:D:115:HIS:CE1	1:W:124:PRO:HB3	2.22	0.74
1:S:6:ARG:NH2	1:S:14:GLU:OE1	2.16	0.74
1:U:6:ARG:NH1	1:U:9:TYR:O	2.20	0.74
1:P:128:ASP:HB2	1:U:131:GLU:HG2	1.68	0.74
1:R:6:ARG:NH2	1:R:14:GLU:OE1	2.18	0.74
1:S:57:HIS:HB3	3:S:259:HOH:O	1.87	0.73
1:A:20:MET:HE1	1:A:111:LEU:N	2.03	0.73
1:T:57:HIS:HB3	3:T:381:HOH:O	1.86	0.73
1:S:152:LEU:HD12	1:S:157:LEU:HD13	1.69	0.73
1:K:60:ARG:CD	1:W:60:ARG:HD3	2.18	0.73
1:B:60:ARG:CD	1:F:60:ARG:HD2	2.19	0.73
1:X:6:ARG:NH2	1:X:14:GLU:OE1	2.20	0.72
1:W:6:ARG:NH2	1:W:14:GLU:OE1	2.22	0.72
1:U:58:GLU:HG2	3:U:187:HOH:O	1.89	0.72
1:P:6:ARG:NH2	1:P:14:GLU:OE1	2.22	0.72
1:U:6:ARG:NH2	1:U:14:GLU:OE1	2.23	0.71
1:H:5:VAL:HG22	1:X:142:ILE:HG22	1.71	0.71
1:D:127:CYS:SG	2:D:191:CU:CU	1.81	0.71
1:S:11:SER:HB2	3:S:250:HOH:O	1.91	0.71
1:D:85:PRO:HG2	3:D:403:HOH:O	1.91	0.70
1:P:173:LYS:HD3	1:P:173:LYS:N	2.03	0.70
1:Q:57:HIS:HB3	3:Q:234:HOH:O	1.90	0.70
1:X:173:LYS:H	1:X:173:LYS:HE3	1.56	0.70
3:N:178:HOH:O	1:R:57:HIS:HB3	1.91	0.70
1:V:144:ARG:HD3	3:V:672:HOH:O	1.92	0.70
1:J:47:ASN:HB2	1:J:168:ASP:OD1	1.91	0.70
1:B:173:LYS:HE2	1:B:173:LYS:H	1.56	0.70
1:G:6:ARG:NH2	1:G:14:GLU:OE1	2.19	0.69
1:V:152:LEU:HD12	1:V:157:LEU:HD13	1.73	0.69
1:F:122:VAL:HG13	3:F:627:HOH:O	1.92	0.69
1:N:154:ARG:NH2	1:U:43:VAL:O	2.24	0.69
1:A:20:MET:HE1	1:A:110:ALA:C	2.14	0.69
1:P:19:ARG:HD3	3:P:346:HOH:O	1.92	0.68
1:P:60:ARG:NE	1:T:60:ARG:HD3	2.07	0.68
1:I:60:ARG:HD2	3:I:179:HOH:O	1.93	0.68
1:O:4:GLN:HG2	3:O:187:HOH:O	1.94	0.68
1:J:51:PHE:HB2	1:J:172:VAL:HG21	1.76	0.68
1:G:148:PHE:O	1:G:152:LEU:HD22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:CE	1:B:110:ALA:HB1	2.24	0.67
1:A:123:ASP:OD2	3:A:746:HOH:O	2.12	0.67
1:Q:60:ARG:HD3	1:U:60:ARG:HD2	1.76	0.67
1:D:127:CYS:SG	2:D:192:CU:CU	1.85	0.67
1:J:152:LEU:HD12	1:J:157:LEU:HD13	1.77	0.66
1:V:6:ARG:NH2	1:V:14:GLU:OE1	2.19	0.66
1:J:5:VAL:HG22	1:Q:142:ILE:HG22	1.77	0.66
1:A:131:GLU:HG2	1:X:128:ASP:HB2	1.77	0.66
1:C:55:HIS:NE2	1:C:104:GLU:OE2	2.28	0.66
1:T:43:VAL:O	1:U:154:ARG:NH2	2.22	0.66
1:C:6:ARG:NH1	1:C:9:TYR:O	2.29	0.66
1:V:137:GLU:HG3	3:V:557:HOH:O	1.96	0.65
1:H:57:HIS:HB3	3:H:648:HOH:O	1.96	0.65
1:W:24:GLU:OE1	1:W:59:GLU:OE1	2.15	0.65
1:M:20:MET:HE2	1:M:20:MET:HA	1.79	0.65
1:C:60:ARG:CD	1:O:60:ARG:HD2	2.27	0.65
1:F:23:LEU:HD13	1:F:107:VAL:HG22	1.79	0.65
1:D:172:VAL:O	1:D:173:LYS:HG3	1.97	0.65
1:D:6:ARG:NH1	1:D:9:TYR:O	2.30	0.65
1:N:64:GLU:OE1	1:R:57:HIS:CE1	2.50	0.64
1:E:154:ARG:NH2	1:L:43:VAL:O	2.29	0.64
1:A:57:HIS:CE1	1:G:64:GLU:OE2	2.50	0.64
1:B:47:ASN:HB3	1:B:172:VAL:HG23	1.78	0.64
1:G:144:ARG:HG2	1:G:144:ARG:HH11	1.62	0.64
1:J:6:ARG:NH2	1:J:14:GLU:OE1	2.26	0.63
1:O:45:LEU:HD13	1:R:154:ARG:NH2	2.14	0.63
1:G:124:PRO:HB3	1:O:115:HIS:CE1	2.33	0.63
1:U:144:ARG:HD3	3:U:200:HOH:O	1.98	0.63
1:J:24:GLU:OE1	1:J:59:GLU:OE1	2.16	0.63
1:F:57:HIS:HB3	3:F:379:HOH:O	1.98	0.62
1:C:142:ILE:HG22	1:S:5:VAL:CG2	2.27	0.62
1:L:122:VAL:O	1:L:122:VAL:CG1	2.48	0.62
1:E:6:ARG:NH1	1:E:9:TYR:O	2.32	0.62
1:F:6:ARG:NH2	1:F:14:GLU:OE1	2.27	0.62
1:B:20:MET:HE3	1:B:110:ALA:C	2.20	0.62
1:T:169:LYS:HG2	1:U:170:HIS:HB3	1.81	0.62
1:B:5:VAL:HG22	1:V:142:ILE:HG13	1.82	0.61
1:M:60:ARG:HD2	1:S:60:ARG:CZ	2.31	0.61
1:U:23:LEU:HD13	1:U:107:VAL:HG22	1.82	0.61
1:S:43:VAL:O	1:T:154:ARG:NH2	2.27	0.61
1:K:60:ARG:HD3	1:W:60:ARG:CD	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:HD2	1:I:60:ARG:CD	2.31	0.61
1:W:20:MET:HE3	1:W:111:LEU:HA	1.81	0.61
1:G:144:ARG:NH1	1:G:144:ARG:HG2	2.15	0.61
1:M:20:MET:HE2	1:M:20:MET:CA	2.31	0.60
1:X:114:LEU:HG	1:X:130:LEU:HD21	1.83	0.60
1:M:124:PRO:HA	1:M:127:CYS:HB3	1.84	0.60
1:S:11:SER:CB	3:S:250:HOH:O	2.49	0.60
1:M:20:MET:CE	1:M:110:ALA:HB1	2.32	0.60
1:E:6:ARG:NH2	1:E:14:GLU:OE1	2.33	0.60
1:E:157:LEU:HD21	1:E:164:GLU:HG3	1.83	0.60
1:B:20:MET:HE1	1:B:110:ALA:HB1	1.84	0.59
1:C:114:LEU:HG	1:C:130:LEU:HD21	1.83	0.59
1:M:83:LYS:HE3	3:M:341:HOH:O	2.02	0.59
1:S:157:LEU:HD21	1:S:164:GLU:HG3	1.83	0.59
1:T:157:LEU:HD21	1:T:164:GLU:HG3	1.83	0.59
1:D:20:MET:HE1	1:D:110:ALA:HB1	1.83	0.59
1:D:43:VAL:O	1:X:154:ARG:NH2	2.32	0.59
1:A:60:ARG:CD	1:G:60:ARG:HE	2.15	0.59
1:E:60:ARG:HD2	1:I:60:ARG:HD3	1.85	0.59
1:A:6:ARG:NH1	1:A:9:TYR:O	2.34	0.59
1:J:154:ARG:NH2	1:R:45:LEU:HD13	2.17	0.59
1:Q:152:LEU:HD13	1:Q:167:PHE:CD1	2.38	0.59
1:I:29:TYR:O	1:I:32:SER:HB3	2.03	0.58
1:A:64:GLU:OE1	1:G:57:HIS:HE1	1.85	0.58
1:C:55:HIS:CE1	1:C:104:GLU:OE2	2.57	0.58
1:L:154:ARG:NH2	1:P:43:VAL:O	2.36	0.58
1:N:60:ARG:HD2	1:R:60:ARG:HD3	1.85	0.58
1:T:45:LEU:HD13	1:U:154:ARG:NH2	2.18	0.58
1:O:43:VAL:O	1:R:154:ARG:NH2	2.24	0.58
3:E:708:HOH:O	1:I:4:GLN:HG2	2.03	0.58
1:E:61:GLU:HG3	3:E:532:HOH:O	2.03	0.58
1:B:43:VAL:O	1:G:154:ARG:NH2	2.30	0.58
1:H:173:LYS:HB3	3:H:635:HOH:O	2.03	0.58
1:W:62:HIS:HB3	1:W:134:TYR:HE2	1.68	0.57
1:S:6:ARG:NH1	1:S:9:TYR:O	2.36	0.57
1:O:98:GLN:HG2	1:O:149:ILE:HD13	1.86	0.57
1:L:142:ILE:HG22	1:T:5:VAL:HG22	1.85	0.57
1:E:20:MET:HE1	1:E:110:ALA:HB1	1.87	0.57
1:D:152:LEU:HD13	1:D:167:PHE:CD1	2.39	0.57
1:C:21:LEU:O	1:C:21:LEU:HD23	2.03	0.57
1:A:114:LEU:HG	1:A:130:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:O	1:F:154:ARG:NH2	2.28	0.57
1:N:20:MET:HE1	1:N:110:ALA:C	2.25	0.57
1:I:21:LEU:HD23	1:I:21:LEU:C	2.25	0.57
1:E:122:VAL:HG12	1:E:122:VAL:O	2.03	0.57
1:W:29:TYR:O	1:W:32:SER:HB3	2.05	0.57
1:K:154:ARG:NH2	1:Q:45:LEU:HD13	2.20	0.57
1:B:126:LEU:O	1:B:130:LEU:HD22	2.05	0.56
1:F:142:ILE:HG22	1:O:5:VAL:HG22	1.87	0.56
1:X:152:LEU:HD12	1:X:157:LEU:HD13	1.87	0.56
1:R:65:LYS:HB3	1:R:134:TYR:OH	2.05	0.56
1:L:20:MET:HE1	1:L:111:LEU:N	2.21	0.56
1:N:45:LEU:HD13	1:S:154:ARG:NH2	2.21	0.56
1:K:84:LYS:HE3	3:W:187:HOH:O	2.06	0.55
3:D:189:HOH:O	1:X:154:ARG:HG3	2.05	0.55
1:S:80:GLN:NE2	1:S:80:GLN:HA	2.21	0.55
1:E:45:LEU:HD13	1:W:154:ARG:NH2	2.22	0.55
1:S:84:LYS:HE2	3:S:180:HOH:O	2.06	0.55
1:E:162:MET:SD	1:W:162:MET:CE	2.95	0.55
1:W:20:MET:HE3	1:W:111:LEU:CA	2.37	0.54
1:N:20:MET:HE1	1:N:111:LEU:N	2.21	0.54
1:B:60:ARG:HD2	3:B:179:HOH:O	2.07	0.54
1:D:60:ARG:HD3	1:H:60:ARG:HD3	1.90	0.54
1:L:2:VAL:HG22	1:L:3:SER:H	1.72	0.54
1:X:20:MET:HE3	1:X:111:LEU:HA	1.89	0.54
1:B:21:LEU:C	1:B:21:LEU:HD23	2.27	0.54
1:X:157:LEU:HD21	1:X:164:GLU:HG3	1.89	0.54
1:J:60:ARG:HD2	1:X:60:ARG:CZ	2.38	0.54
1:B:115:HIS:CE1	1:E:124:PRO:HB3	2.42	0.54
1:M:20:MET:HE3	1:M:110:ALA:HB1	1.89	0.54
1:L:48:VAL:HG23	1:L:168:ASP:OD1	2.08	0.54
1:X:173:LYS:HE3	1:X:173:LYS:N	2.23	0.54
1:Q:64:GLU:OE2	1:U:57:HIS:CE1	2.61	0.54
1:O:173:LYS:HA	1:O:173:LYS:HE3	1.89	0.54
1:M:20:MET:CE	1:M:20:MET:HA	2.37	0.54
1:V:148:PHE:O	1:V:152:LEU:CD2	2.54	0.53
1:N:147:ASP:OD1	1:U:41:ASP:HA	2.08	0.53
1:V:20:MET:HE1	1:V:110:ALA:C	2.29	0.53
1:K:152:LEU:HD13	1:K:167:PHE:CD1	2.44	0.53
1:Q:21:LEU:HD11	1:Q:67:MET:HG3	1.89	0.53
1:V:24:GLU:OE1	1:V:59:GLU:OE1	2.27	0.53
1:H:6:ARG:NH1	1:H:9:TYR:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:VAL:HG22	1:O:142:ILE:HG22	1.90	0.53
1:A:57:HIS:HE1	1:G:64:GLU:OE2	1.89	0.53
1:B:20:MET:HE3	1:B:110:ALA:HB1	1.89	0.53
1:T:148:PHE:O	1:T:152:LEU:HD23	2.10	0.52
1:E:142:ILE:HG22	1:V:5:VAL:HG22	1.91	0.52
1:D:157:LEU:HD21	1:D:164:GLU:HG3	1.92	0.52
1:J:60:ARG:HD2	1:X:60:ARG:NE	2.24	0.52
1:E:23:LEU:HD13	1:E:107:VAL:HG22	1.92	0.52
1:G:6:ARG:NH1	1:G:9:TYR:O	2.42	0.52
1:T:148:PHE:O	1:T:152:LEU:CD2	2.57	0.52
1:G:43:VAL:O	1:H:154:ARG:NH2	2.36	0.52
1:H:6:ARG:NH2	1:H:14:GLU:OE1	2.29	0.52
1:Q:47:ASN:HB2	1:Q:168:ASP:OD1	2.10	0.51
1:T:6:ARG:NH1	1:T:9:TYR:O	2.37	0.51
1:P:57:HIS:HB3	3:P:393:HOH:O	2.10	0.51
1:W:20:MET:HE3	1:W:111:LEU:N	2.25	0.51
1:L:114:LEU:HG	1:L:130:LEU:HD21	1.91	0.51
1:V:108:ASN:O	1:V:111:LEU:HB2	2.11	0.51
1:C:64:GLU:OE2	1:O:57:HIS:CE1	2.63	0.51
1:E:79:LEU:CD1	1:I:33:SER:HB2	2.40	0.51
1:C:21:LEU:C	1:C:21:LEU:HD23	2.31	0.51
1:D:19:ARG:HB3	3:D:615:HOH:O	2.10	0.51
1:C:94:LEU:O	1:C:98:GLN:HG3	2.11	0.51
1:O:24:GLU:OE1	1:O:59:GLU:OE1	2.29	0.51
1:L:39:ASP:HB3	1:V:71:ASN:ND2	2.26	0.51
1:A:43:VAL:O	1:O:154:ARG:NH2	2.39	0.51
1:F:47:ASN:HB3	1:F:172:VAL:HG12	1.93	0.50
1:X:20:MET:HE3	1:X:111:LEU:N	2.26	0.50
1:F:6:ARG:NH1	1:F:9:TYR:O	2.39	0.50
1:P:114:LEU:HG	1:P:130:LEU:HD21	1.93	0.50
1:D:124:PRO:HB3	1:I:115:HIS:CE1	2.47	0.50
1:E:55:HIS:NE2	1:E:104:GLU:OE2	2.43	0.50
1:V:60:ARG:HH11	1:V:60:ARG:HG3	1.76	0.50
1:Q:71:ASN:ND2	1:U:39:ASP:HB3	2.26	0.50
1:M:115:HIS:NE2	1:M:131:GLU:OE2	2.38	0.50
1:A:60:ARG:CD	1:G:60:ARG:NE	2.62	0.50
1:C:93:THR:HG22	1:C:152:LEU:HD21	1.94	0.50
1:K:60:ARG:NH1	1:W:60:ARG:HD3	2.26	0.50
1:V:142:ILE:HG12	1:V:143:LYS:N	2.27	0.50
1:M:98:GLN:HG2	1:M:149:ILE:HD13	1.93	0.50
1:W:102:GLN:HB2	3:W:683:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:LYS:HD2	1:K:57:HIS:CE1	2.46	0.49
3:J:180:HOH:O	1:X:57:HIS:HB3	2.11	0.49
1:L:24:GLU:OE1	1:L:59:GLU:OE1	2.30	0.49
1:B:60:ARG:HD3	1:F:60:ARG:HD2	1.93	0.49
1:N:25:LEU:HB3	1:N:82:ILE:HD13	1.93	0.49
1:R:6:ARG:NH1	1:R:9:TYR:O	2.43	0.49
1:H:173:LYS:NZ	1:H:173:LYS:H	2.10	0.49
1:O:157:LEU:HD21	1:O:164:GLU:HG3	1.95	0.49
1:E:126:LEU:O	1:E:130:LEU:HD22	2.12	0.49
1:F:124:PRO:HB3	1:G:115:HIS:CE1	2.47	0.49
1:S:118:ALA:HB2	1:S:126:LEU:CD2	2.37	0.49
1:K:60:ARG:HD2	3:W:188:HOH:O	2.11	0.49
1:E:115:HIS:CE1	1:V:124:PRO:HG3	2.47	0.49
1:A:79:LEU:HD12	1:G:33:SER:HB2	1.95	0.49
1:H:45:LEU:HD13	1:I:154:ARG:NH2	2.27	0.49
1:P:21:LEU:HD23	1:P:21:LEU:C	2.33	0.49
1:D:24:GLU:OE1	1:D:59:GLU:OE1	2.30	0.49
1:N:65:LYS:HE2	1:N:133:GLU:OE1	2.13	0.49
1:T:114:LEU:HG	1:T:130:LEU:HD21	1.94	0.49
1:L:20:MET:HE1	1:L:110:ALA:C	2.32	0.48
1:F:37:PHE:O	1:F:40:ARG:HB2	2.12	0.48
1:C:124:PRO:HB3	1:R:115:HIS:CE1	2.48	0.48
1:N:60:ARG:CD	1:R:60:ARG:HD3	2.42	0.48
1:K:57:HIS:HB3	3:W:772:HOH:O	2.12	0.48
1:I:93:THR:HG22	1:I:152:LEU:HD21	1.95	0.48
1:I:114:LEU:HG	1:I:130:LEU:HD21	1.95	0.48
1:N:114:LEU:HG	1:N:130:LEU:HD21	1.94	0.48
1:X:60:ARG:NH2	3:X:537:HOH:O	2.46	0.48
1:L:6:ARG:HD3	3:L:465:HOH:O	2.13	0.48
1:Q:60:ARG:HD2	3:Q:568:HOH:O	2.13	0.48
1:S:45:LEU:HD13	1:T:154:ARG:NH2	2.29	0.48
1:L:20:MET:CE	1:L:111:LEU:HD23	2.44	0.48
1:O:95:GLU:HG3	3:O:383:HOH:O	2.13	0.48
1:B:157:LEU:HD11	1:B:164:GLU:HG3	1.95	0.48
1:N:35:TYR:CE1	1:N:53:LYS:HD3	2.49	0.48
1:H:86:GLU:HB2	3:H:189:HOH:O	2.11	0.48
1:J:24:GLU:HB2	1:J:63:ALA:HB2	1.96	0.48
1:K:21:LEU:C	1:K:21:LEU:HD23	2.34	0.48
1:V:62:HIS:HB3	1:V:134:TYR:HE2	1.79	0.48
1:L:53:LYS:HE3	1:V:64:GLU:OE2	2.14	0.48
1:C:20:MET:HE1	1:C:110:ALA:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:69:TYR:HE1	1:S:125:HIS:CE1	2.32	0.47
1:K:29:TYR:O	1:K:32:SER:HB2	2.14	0.47
1:O:152:LEU:HD12	1:O:157:LEU:HD13	1.96	0.47
1:D:114:LEU:HG	1:D:130:LEU:HD21	1.96	0.47
1:A:20:MET:CE	1:A:110:ALA:C	2.80	0.47
1:L:60:ARG:CZ	1:V:60:ARG:HD3	2.44	0.47
1:W:65:LYS:HE2	1:W:133:GLU:OE1	2.14	0.47
1:N:57:HIS:HB3	3:N:734:HOH:O	2.13	0.47
1:M:60:ARG:HD2	1:S:60:ARG:NH1	2.29	0.47
1:A:154:ARG:NH2	1:J:45:LEU:HD13	2.28	0.47
1:U:21:LEU:C	1:U:21:LEU:HD23	2.35	0.47
1:X:20:MET:HE3	1:X:110:ALA:C	2.34	0.47
1:S:69:TYR:CE1	1:S:125:HIS:CE1	3.02	0.47
1:I:85:PRO:HG2	3:I:186:HOH:O	2.15	0.47
1:W:152:LEU:HD12	1:W:157:LEU:HD13	1.97	0.47
1:T:127:CYS:SG	1:T:131:GLU:OE2	2.73	0.47
1:S:118:ALA:CB	1:S:126:LEU:HD23	2.35	0.47
1:E:162:MET:SD	1:W:162:MET:HE1	2.55	0.47
1:Q:16:ALA:HB1	1:Q:114:LEU:HD13	1.96	0.47
3:A:179:HOH:O	1:X:122:VAL:HG12	2.15	0.47
1:K:20:MET:HE1	1:K:110:ALA:C	2.34	0.47
1:L:148:PHE:O	1:L:152:LEU:HD22	2.14	0.47
1:M:157:LEU:HD11	1:M:164:GLU:HG3	1.96	0.47
1:G:27:ALA:HA	1:G:103:LEU:HD21	1.96	0.47
1:F:135:LEU:O	1:F:139:VAL:HG13	2.15	0.47
1:M:20:MET:HE1	1:M:110:ALA:HB1	1.97	0.46
1:I:24:GLU:OE1	1:I:59:GLU:OE1	2.33	0.46
1:K:6:ARG:NH1	1:K:9:TYR:O	2.38	0.46
1:K:173:LYS:HE3	1:K:173:LYS:C	2.35	0.46
1:R:101:LEU:HD22	1:R:149:ILE:HD12	1.96	0.46
1:G:2:VAL:N	3:G:190:HOH:O	2.48	0.46
1:P:20:MET:HE1	1:P:110:ALA:C	2.36	0.46
1:W:16:ALA:HB1	1:W:114:LEU:HD13	1.97	0.46
1:E:165:TYR:CD2	1:W:155:LEU:HD21	2.51	0.46
1:K:79:LEU:HD12	1:W:33:SER:HB2	1.96	0.46
1:S:46:HIS:O	1:S:49:ALA:HB3	2.16	0.46
1:K:124:PRO:HB3	1:P:115:HIS:CE1	2.51	0.46
3:Q:178:HOH:O	1:U:4:GLN:HG2	2.15	0.46
1:B:60:ARG:NE	1:F:60:ARG:HD2	2.30	0.46
1:O:57:HIS:HB3	3:O:188:HOH:O	2.16	0.46
1:B:6:ARG:NH1	1:B:9:TYR:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:LEU:HD22	1:I:163:GLY:HA2	1.98	0.46
1:M:10:HIS:CD2	1:M:121:LYS:HE3	2.51	0.46
1:R:135:LEU:HA	1:R:135:LEU:HD12	1.84	0.46
1:B:79:LEU:HD12	1:F:33:SER:HB2	1.96	0.46
1:U:57:HIS:HB3	3:U:287:HOH:O	2.15	0.45
1:U:114:LEU:HD23	1:U:130:LEU:HD11	1.98	0.45
1:O:114:LEU:HG	1:O:130:LEU:HD21	1.98	0.45
1:G:140:LYS:HB2	1:G:140:LYS:HE3	1.69	0.45
1:W:37:PHE:O	1:W:40:ARG:HB2	2.15	0.45
1:Q:33:SER:HB2	1:U:79:LEU:HD12	1.98	0.45
1:N:131:GLU:HG2	1:Q:128:ASP:HB2	1.98	0.45
1:G:148:PHE:O	1:G:152:LEU:CD2	2.62	0.45
1:H:41:ASP:HA	1:I:147:ASP:OD1	2.17	0.45
1:J:154:ARG:NH2	1:R:45:LEU:CD1	2.79	0.45
1:H:173:LYS:H	1:H:173:LYS:HZ3	1.64	0.45
1:V:127:CYS:SG	1:V:131:GLU:OE2	2.74	0.45
1:K:131:GLU:HB3	1:U:128:ASP:HB2	1.99	0.45
1:T:42:ASP:HA	1:U:150:THR:OG1	2.17	0.45
1:M:75:GLY:O	1:M:76:ARG:NH1	2.47	0.45
3:N:177:HOH:O	1:R:60:ARG:HD2	2.16	0.45
1:I:21:LEU:HD23	1:I:21:LEU:O	2.16	0.45
1:D:60:ARG:NH1	1:H:60:ARG:HD2	2.31	0.45
1:L:124:PRO:HB3	1:M:115:HIS:CE1	2.52	0.45
1:P:21:LEU:HD11	1:P:67:MET:HG2	1.98	0.45
1:I:152:LEU:HD13	1:I:167:PHE:CD1	2.52	0.45
1:E:115:HIS:ND1	1:V:124:PRO:HG3	2.32	0.45
1:J:16:ALA:HB1	1:J:114:LEU:HD13	1.99	0.45
1:P:173:LYS:N	1:P:173:LYS:CD	2.67	0.44
1:L:118:ALA:HB2	1:L:126:LEU:HD23	1.99	0.44
1:F:10:HIS:CG	1:F:121:LYS:HD2	2.52	0.44
1:R:73:ARG:HD2	1:R:73:ARG:HA	1.77	0.44
1:K:60:ARG:CZ	1:W:60:ARG:HD3	2.48	0.44
1:N:79:LEU:HD12	1:R:33:SER:HB2	1.99	0.44
1:W:114:LEU:HG	1:W:130:LEU:HD21	1.99	0.44
1:C:144:ARG:HD2	3:C:177:HOH:O	2.16	0.44
1:F:16:ALA:HB1	1:F:114:LEU:HD13	1.99	0.44
1:E:24:GLU:OE1	1:E:59:GLU:OE1	2.34	0.44
1:A:60:ARG:HD3	1:G:60:ARG:CZ	2.44	0.44
1:P:79:LEU:HD13	1:T:29:TYR:CE1	2.52	0.44
1:H:69:TYR:CE2	1:H:126:LEU:HD13	2.52	0.44
1:G:160:ASN:OD1	1:G:160:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:LEU:HD23	1:L:112:LEU:HA	1.84	0.44
1:T:75:GLY:O	1:T:76:ARG:NH1	2.51	0.44
1:A:64:GLU:OE1	1:G:57:HIS:CE1	2.69	0.44
1:I:5:VAL:HG22	1:W:142:ILE:HG22	1.98	0.44
1:S:114:LEU:HG	1:S:130:LEU:HD21	1.98	0.44
1:V:23:LEU:O	1:V:26:TYR:HB3	2.17	0.44
1:Q:140:LYS:HB2	1:Q:140:LYS:HE3	1.72	0.44
1:C:25:LEU:HA	1:C:25:LEU:HD23	1.85	0.44
1:D:60:ARG:HD3	1:H:60:ARG:CD	2.48	0.44
1:C:60:ARG:HD3	1:O:60:ARG:CD	2.36	0.43
1:B:154:ARG:NH2	1:I:45:LEU:HD13	2.33	0.43
1:V:46:HIS:CE1	1:V:50:GLU:OE2	2.71	0.43
1:E:79:LEU:HD12	1:I:33:SER:HB2	2.00	0.43
1:J:124:PRO:HB3	1:Q:115:HIS:CE1	2.53	0.43
1:H:124:PRO:HB3	1:X:115:HIS:CE1	2.53	0.43
1:C:116:LYS:HD3	1:S:122:VAL:HG11	2.00	0.43
1:B:20:MET:HE3	1:B:110:ALA:CB	2.49	0.43
1:C:57:HIS:HE1	1:O:64:GLU:OE1	2.00	0.43
1:K:35:TYR:CD1	1:K:53:LYS:HB2	2.53	0.43
1:M:6:ARG:NH1	1:M:9:TYR:O	2.38	0.43
1:P:33:SER:HB2	1:T:79:LEU:HD12	2.01	0.43
1:N:115:HIS:CE1	1:Q:124:PRO:HB3	2.54	0.43
1:O:47:ASN:HB3	1:O:172:VAL:HG23	1.99	0.43
1:M:145:ILE:O	1:M:149:ILE:HG13	2.17	0.43
1:M:125:HIS:CD2	1:T:139:VAL:HG13	2.53	0.43
1:H:73:ARG:HA	1:H:73:ARG:HD2	1.50	0.43
1:E:16:ALA:HB1	1:E:114:LEU:HD13	2.00	0.43
1:E:20:MET:HE3	1:E:110:ALA:O	2.18	0.43
1:D:136:GLU:OE2	1:W:72:LYS:NZ	2.52	0.43
1:R:124:PRO:HB3	1:S:115:HIS:CE1	2.54	0.43
1:U:73:ARG:HD2	1:U:73:ARG:HA	1.59	0.43
1:B:24:GLU:OE1	1:B:59:GLU:OE1	2.37	0.43
1:K:127:CYS:SG	1:P:131:GLU:OE1	2.77	0.43
1:K:5:VAL:HG22	1:P:142:ILE:HG22	2.00	0.43
1:U:20:MET:O	1:U:24:GLU:HG2	2.19	0.43
1:W:21:LEU:HD11	1:W:67:MET:HG2	2.00	0.43
1:M:125:HIS:CD2	1:T:139:VAL:CG1	3.02	0.42
1:O:86:GLU:HG2	3:O:709:HOH:O	2.18	0.42
1:C:37:PHE:CD2	1:C:90:TRP:HB2	2.54	0.42
1:G:130:LEU:HA	1:G:130:LEU:HD12	1.88	0.42
1:N:73:ARG:HA	1:N:73:ARG:HD2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:LEU:HD12	1:F:130:LEU:HA	1.86	0.42
1:E:168:ASP:OD2	1:E:169:LYS:HD3	2.18	0.42
1:A:165:TYR:CD2	1:O:155:LEU:HD21	2.54	0.42
1:P:152:LEU:HD13	1:P:167:PHE:CD1	2.53	0.42
1:J:33:SER:HB2	1:X:79:LEU:HD12	2.01	0.42
1:C:173:LYS:HZ2	1:C:173:LYS:HB3	1.84	0.42
1:O:60:ARG:NH1	3:O:178:HOH:O	2.52	0.42
1:P:60:ARG:CD	1:T:60:ARG:HD3	2.49	0.42
1:F:16:ALA:CB	1:F:114:LEU:HD13	2.50	0.42
1:F:23:LEU:CD1	1:F:107:VAL:HG22	2.48	0.42
1:W:20:MET:CE	1:W:111:LEU:HD23	2.49	0.42
1:W:4:GLN:HB2	3:W:363:HOH:O	2.19	0.42
1:C:135:LEU:HD21	1:S:124:PRO:HB2	2.01	0.42
1:W:20:MET:HE3	1:W:111:LEU:HD23	2.01	0.42
1:M:86:GLU:HB2	3:M:186:HOH:O	2.19	0.42
1:A:115:HIS:CE1	1:X:124:PRO:HB3	2.55	0.42
1:K:30:THR:OG1	1:K:85:PRO:HB3	2.19	0.42
1:E:124:PRO:HA	1:E:127:CYS:HB3	2.01	0.41
1:B:9:TYR:CE2	1:B:14:GLU:HB2	2.55	0.41
1:B:144:ARG:O	1:B:147:ASP:HB2	2.20	0.41
1:H:25:LEU:HA	1:H:25:LEU:HD23	1.83	0.41
1:J:41:ASP:OD2	1:X:4:GLN:HG2	2.20	0.41
1:Q:21:LEU:HD23	1:Q:21:LEU:C	2.41	0.41
1:M:162:MET:O	1:M:165:TYR:HB3	2.19	0.41
1:W:101:LEU:O	1:W:105:LYS:HG3	2.19	0.41
1:I:35:TYR:CD1	1:I:53:LYS:HB2	2.55	0.41
1:K:33:SER:HB2	1:W:79:LEU:HD12	2.02	0.41
1:M:154:ARG:NH2	1:V:45:LEU:HD13	2.34	0.41
1:N:60:ARG:NE	1:R:60:ARG:HH11	2.19	0.41
1:K:84:LYS:HD2	3:W:518:HOH:O	2.20	0.41
1:O:73:ARG:HA	1:O:73:ARG:HD2	1.69	0.41
1:P:39:ASP:HB3	1:T:71:ASN:ND2	2.35	0.41
1:X:37:PHE:CE1	1:X:89:GLU:HB2	2.55	0.41
1:M:173:LYS:H	1:M:173:LYS:NZ	2.18	0.41
1:L:24:GLU:HA	1:L:24:GLU:OE1	2.21	0.41
1:K:21:LEU:HD11	1:K:67:MET:HG2	2.03	0.41
1:J:114:LEU:HG	1:J:130:LEU:HD21	2.02	0.41
1:V:10:HIS:CD2	1:V:121:LYS:HE3	2.54	0.41
1:E:75:GLY:O	1:E:76:ARG:NH1	2.53	0.41
1:H:47:ASN:O	1:H:172:VAL:HG11	2.21	0.41
1:K:73:ARG:HD2	1:K:73:ARG:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:47:ASN:HB3	1:K:172:VAL:HG13	2.02	0.41
1:W:23:LEU:HA	1:W:23:LEU:HD23	1.94	0.41
1:W:135:LEU:HA	1:W:135:LEU:HD12	1.90	0.41
1:M:60:ARG:NE	1:S:60:ARG:HD2	2.35	0.40
1:S:69:TYR:CE1	1:S:125:HIS:HE1	2.39	0.40
1:Q:24:GLU:OE1	1:Q:59:GLU:OE1	2.38	0.40
1:X:20:MET:HE3	1:X:111:LEU:CA	2.51	0.40
1:K:60:ARG:NH1	1:W:60:ARG:CD	2.85	0.40
1:V:135:LEU:HD12	1:V:135:LEU:HA	1.92	0.40
1:K:20:MET:HG3	1:K:66:PHE:CE2	2.57	0.40
1:T:24:GLU:OE1	1:T:59:GLU:OE1	2.39	0.40
1:G:21:LEU:HD11	1:G:67:MET:HG2	2.03	0.40
1:U:101:LEU:O	1:U:105:LYS:HG3	2.21	0.40
1:V:6:ARG:NH1	1:V:9:TYR:O	2.48	0.40
1:B:73:ARG:HD2	1:B:73:ARG:HA	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
1	B	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	C	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	D	170/176 (97%)	159 (94%)	10 (6%)	1 (1%)	30	63
1	E	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	F	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
1	G	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	H	170/176 (97%)	166 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	J	170/176 (97%)	166 (98%)	3 (2%)	1 (1%)	30	63
1	K	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	L	170/176 (97%)	162 (95%)	8 (5%)	0	100	100
1	M	170/176 (97%)	159 (94%)	10 (6%)	1 (1%)	30	63
1	N	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	O	170/176 (97%)	164 (96%)	5 (3%)	1 (1%)	30	63
1	P	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	Q	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	R	170/176 (97%)	163 (96%)	6 (4%)	1 (1%)	30	63
1	S	170/176 (97%)	167 (98%)	3 (2%)	0	100	100
1	T	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	U	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	V	170/176 (97%)	163 (96%)	5 (3%)	2 (1%)	16	45
1	W	170/176 (97%)	166 (98%)	3 (2%)	1 (1%)	30	63
1	X	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
All	All	4080/4224 (97%)	3937 (96%)	135 (3%)	8 (0%)	52	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	122	VAL
1	D	81	ASP
1	J	122	VAL
1	V	11	SER
1	O	81	ASP
1	V	122	VAL
1	R	122	VAL
1	W	122	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	153/157 (98%)	138 (90%)	15 (10%)	10 28
1	B	153/157 (98%)	135 (88%)	18 (12%)	6 19
1	C	153/157 (98%)	133 (87%)	20 (13%)	5 14
1	D	153/157 (98%)	137 (90%)	16 (10%)	8 24
1	E	153/157 (98%)	134 (88%)	19 (12%)	6 17
1	F	153/157 (98%)	133 (87%)	20 (13%)	5 14
1	G	153/157 (98%)	136 (89%)	17 (11%)	8 22
1	H	153/157 (98%)	133 (87%)	20 (13%)	5 14
1	I	153/157 (98%)	136 (89%)	17 (11%)	8 22
1	J	153/157 (98%)	133 (87%)	20 (13%)	5 14
1	K	153/157 (98%)	137 (90%)	16 (10%)	8 24
1	L	153/157 (98%)	135 (88%)	18 (12%)	6 19
1	M	153/157 (98%)	136 (89%)	17 (11%)	8 22
1	N	153/157 (98%)	136 (89%)	17 (11%)	8 22
1	O	153/157 (98%)	136 (89%)	17 (11%)	8 22
1	P	153/157 (98%)	135 (88%)	18 (12%)	6 19
1	Q	153/157 (98%)	132 (86%)	21 (14%)	4 13
1	R	153/157 (98%)	135 (88%)	18 (12%)	6 19
1	S	153/157 (98%)	132 (86%)	21 (14%)	4 13
1	T	153/157 (98%)	137 (90%)	16 (10%)	8 24
1	U	153/157 (98%)	131 (86%)	22 (14%)	4 11
1	V	153/157 (98%)	141 (92%)	12 (8%)	16 40
1	W	153/157 (98%)	140 (92%)	13 (8%)	13 36
1	X	153/157 (98%)	130 (85%)	23 (15%)	3 10
All	All	3672/3768 (98%)	3241 (88%)	431 (12%)	7 20

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	32	SER
1	A	45	LEU
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	68	LYS
1	A	89	GLU
1	A	105	LYS
1	A	116	LYS
1	A	121	LYS
1	A	127	CYS
1	A	130	LEU
1	A	132	SER
1	A	139	VAL
1	A	152	LEU
1	A	171	SER
1	B	5	VAL
1	B	23	LEU
1	B	29	TYR
1	B	45	LEU
1	B	54	GLU
1	B	64	GLU
1	B	68	LYS
1	B	89	GLU
1	B	98	GLN
1	B	116	LYS
1	B	121	LYS
1	B	127	CYS
1	B	130	LEU
1	B	135	LEU
1	B	136	GLU
1	B	152	LEU
1	B	157	LEU
1	B	173	LYS
1	C	5	VAL
1	C	11	SER
1	C	23	LEU
1	C	29	TYR
1	C	32	SER
1	C	45	LEU
1	C	54	GLU
1	C	84	LYS
1	C	121	LYS
1	C	122	VAL
1	C	127	CYS
1	C	128	ASP
1	C	130	LEU

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Mol	Chain	Res	Type
1	C	135	LEU
1	C	137	GLU
1	C	139	VAL
1	C	144	ARG
1	C	152	LEU
1	C	172	VAL
1	C	173	LYS
1	D	11	SER
1	D	21	LEU
1	D	23	LEU
1	D	29	TYR
1	D	45	LEU
1	D	55	HIS
1	D	60	ARG
1	D	65	LYS
1	D	68	LYS
1	D	130	LEU
1	D	135	LEU
1	D	139	VAL
1	D	140	LYS
1	D	144	ARG
1	D	152	LEU
1	D	172	VAL
1	E	2	VAL
1	E	23	LEU
1	E	28	SER
1	E	29	TYR
1	E	32	SER
1	E	45	LEU
1	E	55	HIS
1	E	60	ARG
1	E	61	GLU
1	E	68	LYS
1	E	84	LYS
1	E	121	LYS
1	E	130	LEU
1	E	135	LEU
1	E	137	GLU
1	E	139	VAL
1	E	140	LYS
1	E	152	LEU
1	E	157	LEU

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Mol	Chain	Res	Type
1	F	23	LEU
1	F	29	TYR
1	F	32	SER
1	F	41	ASP
1	F	45	LEU
1	F	54	GLU
1	F	55	HIS
1	F	61	GLU
1	F	68	LYS
1	F	86	GLU
1	F	89	GLU
1	F	102	GLN
1	F	119	THR
1	F	122	VAL
1	F	127	CYS
1	F	130	LEU
1	F	137	GLU
1	F	140	LYS
1	F	144	ARG
1	F	152	LEU
1	G	11	SER
1	G	23	LEU
1	G	29	TYR
1	G	45	LEU
1	G	54	GLU
1	G	55	HIS
1	G	60	ARG
1	G	61	GLU
1	G	98	GLN
1	G	130	LEU
1	G	135	LEU
1	G	137	GLU
1	G	139	VAL
1	G	144	ARG
1	G	152	LEU
1	G	157	LEU
1	G	173	LYS
1	H	2	VAL
1	H	3	SER
1	H	6	ARG
1	H	23	LEU
1	H	29	TYR

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Mol	Chain	Res	Type
1	H	45	LEU
1	H	55	HIS
1	H	64	GLU
1	H	83	LYS
1	H	89	GLU
1	H	116	LYS
1	H	121	LYS
1	H	122	VAL
1	H	127	CYS
1	H	130	LEU
1	H	135	LEU
1	H	139	VAL
1	H	152	LEU
1	H	171	SER
1	H	173	LYS
1	I	2	VAL
1	I	5	VAL
1	I	23	LEU
1	I	29	TYR
1	I	33	SER
1	I	45	LEU
1	I	89	GLU
1	I	98	GLN
1	I	116	LYS
1	I	121	LYS
1	I	130	LEU
1	I	135	LEU
1	I	137	GLU
1	I	139	VAL
1	I	152	LEU
1	I	171	SER
1	I	172	VAL
1	J	5	VAL
1	J	11	SER
1	J	21	LEU
1	J	23	LEU
1	J	29	TYR
1	J	32	SER
1	J	45	LEU
1	J	84	LYS
1	J	86	GLU
1	J	102	GLN

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Mol	Chain	Res	Type
1	J	116	LYS
1	J	121	LYS
1	J	122	VAL
1	J	127	CYS
1	J	130	LEU
1	J	135	LEU
1	J	137	GLU
1	J	140	LYS
1	J	152	LEU
1	J	157	LEU
1	K	2	VAL
1	K	19	ARG
1	K	23	LEU
1	K	45	LEU
1	K	53	LYS
1	K	55	HIS
1	K	58	GLU
1	K	119	THR
1	K	121	LYS
1	K	127	CYS
1	K	130	LEU
1	K	135	LEU
1	K	139	VAL
1	K	152	LEU
1	K	168	ASP
1	K	173	LYS
1	L	2	VAL
1	L	23	LEU
1	L	45	LEU
1	L	60	ARG
1	L	84	LYS
1	L	102	GLN
1	L	116	LYS
1	L	117	LEU
1	L	121	LYS
1	L	127	CYS
1	L	130	LEU
1	L	135	LEU
1	L	137	GLU
1	L	139	VAL
1	L	140	LYS
1	L	152	LEU

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Mol	Chain	Res	Type
1	L	171	SER
1	L	172	VAL
1	M	2	VAL
1	M	11	SER
1	M	23	LEU
1	M	29	TYR
1	M	45	LEU
1	M	55	HIS
1	M	65	LYS
1	M	86	GLU
1	M	105	LYS
1	M	116	LYS
1	M	122	VAL
1	M	130	LEU
1	M	137	GLU
1	M	139	VAL
1	M	152	LEU
1	M	172	VAL
1	M	173	LYS
1	N	5	VAL
1	N	23	LEU
1	N	28	SER
1	N	29	TYR
1	N	32	SER
1	N	45	LEU
1	N	65	LYS
1	N	83	LYS
1	N	116	LYS
1	N	121	LYS
1	N	122	VAL
1	N	127	CYS
1	N	130	LEU
1	N	137	GLU
1	N	139	VAL
1	N	152	LEU
1	N	173	LYS
1	O	5	VAL
1	O	11	SER
1	O	20	MET
1	O	23	LEU
1	O	29	TYR
1	O	32	SER

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Mol	Chain	Res	Type
1	O	45	LEU
1	O	54	GLU
1	O	68	LYS
1	O	86	GLU
1	O	127	CYS
1	O	130	LEU
1	O	135	LEU
1	O	137	GLU
1	O	152	LEU
1	O	157	LEU
1	O	173	LYS
1	P	2	VAL
1	P	23	LEU
1	P	29	TYR
1	P	45	LEU
1	P	72	LYS
1	P	86	GLU
1	P	89	GLU
1	P	98	GLN
1	P	102	GLN
1	P	116	LYS
1	P	121	LYS
1	P	127	CYS
1	P	130	LEU
1	P	135	LEU
1	P	139	VAL
1	P	140	LYS
1	P	152	LEU
1	P	173	LYS
1	Q	5	VAL
1	Q	11	SER
1	Q	23	LEU
1	Q	32	SER
1	Q	33	SER
1	Q	45	LEU
1	Q	53	LYS
1	Q	65	LYS
1	Q	68	LYS
1	Q	86	GLU
1	Q	89	GLU
1	Q	98	GLN
1	Q	116	LYS

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Mol	Chain	Res	Type
1	Q	121	LYS
1	Q	122	VAL
1	Q	127	CYS
1	Q	130	LEU
1	Q	135	LEU
1	Q	137	GLU
1	Q	152	LEU
1	Q	172	VAL
1	R	2	VAL
1	R	5	VAL
1	R	21	LEU
1	R	23	LEU
1	R	32	SER
1	R	45	LEU
1	R	65	LYS
1	R	98	GLN
1	R	102	GLN
1	R	119	THR
1	R	121	LYS
1	R	127	CYS
1	R	130	LEU
1	R	135	LEU
1	R	152	LEU
1	R	169	LYS
1	R	172	VAL
1	R	173	LYS
1	S	2	VAL
1	S	5	VAL
1	S	21	LEU
1	S	23	LEU
1	S	28	SER
1	S	29	TYR
1	S	45	LEU
1	S	60	ARG
1	S	68	LYS
1	S	72	LYS
1	S	84	LYS
1	S	98	GLN
1	S	116	LYS
1	S	119	THR
1	S	130	LEU
1	S	139	VAL

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Mol	Chain	Res	Type
1	S	144	ARG
1	S	152	LEU
1	S	157	LEU
1	S	168	ASP
1	S	173	LYS
1	T	5	VAL
1	T	11	SER
1	T	23	LEU
1	T	45	LEU
1	T	65	LYS
1	T	83	LYS
1	T	98	GLN
1	T	116	LYS
1	T	121	LYS
1	T	122	VAL
1	T	130	LEU
1	T	135	LEU
1	T	139	VAL
1	T	140	LYS
1	T	154	ARG
1	T	169	LYS
1	U	2	VAL
1	U	11	SER
1	U	23	LEU
1	U	29	TYR
1	U	41	ASP
1	U	45	LEU
1	U	55	HIS
1	U	68	LYS
1	U	84	LYS
1	U	86	GLU
1	U	116	LYS
1	U	121	LYS
1	U	122	VAL
1	U	127	CYS
1	U	130	LEU
1	U	135	LEU
1	U	137	GLU
1	U	139	VAL
1	U	144	ARG
1	U	152	LEU
1	U	157	LEU

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Mol	Chain	Res	Type
1	U	173	LYS
1	V	11	SER
1	V	23	LEU
1	V	45	LEU
1	V	60	ARG
1	V	68	LYS
1	V	130	LEU
1	V	135	LEU
1	V	139	VAL
1	V	140	LYS
1	V	142	ILE
1	V	157	LEU
1	V	173	LYS
1	W	23	LEU
1	W	45	LEU
1	W	53	LYS
1	W	68	LYS
1	W	84	LYS
1	W	117	LEU
1	W	122	VAL
1	W	130	LEU
1	W	135	LEU
1	W	139	VAL
1	W	152	LEU
1	W	157	LEU
1	W	171	SER
1	X	2	VAL
1	X	5	VAL
1	X	23	LEU
1	X	29	TYR
1	X	32	SER
1	X	45	LEU
1	X	53	LYS
1	X	54	GLU
1	X	55	HIS
1	X	61	GLU
1	X	64	GLU
1	X	116	LYS
1	X	121	LYS
1	X	122	VAL
1	X	130	LEU
1	X	135	LEU

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Mol	Chain	Res	Type
1	X	137	GLU
1	X	139	VAL
1	X	144	ARG
1	X	152	LEU
1	X	157	LEU
1	X	172	VAL
1	X	173	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	98	GLN
1	A	138	GLN
1	B	98	GLN
1	C	57	HIS
1	D	98	GLN
1	D	138	GLN
1	E	71	ASN
1	E	98	GLN
1	E	138	GLN
1	F	98	GLN
1	G	57	HIS
1	G	98	GLN
1	G	138	GLN
1	H	80	GLN
1	H	98	GLN
1	H	138	GLN
1	I	55	HIS
1	I	57	HIS
1	I	98	GLN
1	I	138	GLN
1	J	46	HIS
1	J	138	GLN
1	K	55	HIS
1	K	57	HIS
1	K	80	GLN
1	L	98	GLN
1	L	138	GLN
1	M	57	HIS
1	M	138	GLN
1	N	98	GLN

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Mol	Chain	Res	Type
1	O	57	HIS
1	O	138	GLN
1	P	55	HIS
1	P	98	GLN
1	P	138	GLN
1	Q	98	GLN
1	Q	138	GLN
1	R	98	GLN
1	R	138	GLN
1	S	80	GLN
1	S	98	GLN
1	T	80	GLN
1	T	98	GLN
1	T	138	GLN
1	U	57	HIS
1	U	98	GLN
1	U	138	GLN
1	V	46	HIS
1	V	80	GLN
1	V	138	GLN
1	W	57	HIS
1	W	80	GLN
1	W	98	GLN
1	W	138	GLN
1	X	57	HIS
1	X	138	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 162 ligands modelled in this entry, 162 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	172/176 (97%)	-0.74	0	100	100	22, 32, 46, 54	0
1	B	172/176 (97%)	-0.67	0	100	100	31, 40, 54, 66	0
1	C	172/176 (97%)	-0.78	0	100	100	24, 35, 47, 64	0
1	D	172/176 (97%)	-0.80	0	100	100	21, 31, 48, 57	0
1	E	172/176 (97%)	-0.72	0	100	100	28, 39, 53, 60	0
1	F	172/176 (97%)	-0.66	0	100	100	27, 38, 50, 68	0
1	G	172/176 (97%)	-0.72	0	100	100	27, 36, 47, 68	0
1	H	172/176 (97%)	-0.79	0	100	100	22, 33, 46, 61	0
1	I	172/176 (97%)	-0.69	0	100	100	30, 39, 51, 66	0
1	J	172/176 (97%)	-0.76	0	100	100	19, 29, 44, 63	0
1	K	172/176 (97%)	-0.84	0	100	100	21, 29, 43, 54	0
1	L	172/176 (97%)	-0.74	0	100	100	30, 40, 52, 62	0
1	M	172/176 (97%)	-0.70	0	100	100	30, 40, 52, 61	0
1	N	172/176 (97%)	-0.85	0	100	100	18, 30, 45, 60	0
1	O	172/176 (97%)	-0.80	0	100	100	20, 31, 45, 57	0
1	P	172/176 (97%)	-0.73	0	100	100	26, 35, 47, 62	0
1	Q	172/176 (97%)	-0.80	0	100	100	21, 30, 43, 55	0
1	R	172/176 (97%)	-0.81	0	100	100	19, 31, 46, 61	0
1	S	172/176 (97%)	-0.67	0	100	100	27, 37, 50, 65	0
1	T	172/176 (97%)	-0.74	0	100	100	28, 37, 51, 65	0
1	U	172/176 (97%)	-0.77	0	100	100	22, 32, 45, 65	0
1	V	172/176 (97%)	-0.71	0	100	100	31, 42, 55, 66	0
1	W	172/176 (97%)	-0.81	0	100	100	23, 32, 45, 56	0
1	X	172/176 (97%)	-0.79	0	100	100	20, 29, 43, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	4128/4224 (97%)	-0.75	0	100	100	18, 35, 50, 68	0

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CU	M	182	1/1	0.94	0.19	5.33	63,63,63,63	1
2	CU	H	177	1/1	0.79	0.17	4.39	44,44,44,44	1
2	CU	P	181	1/1	0.91	0.15	2.60	72,72,72,72	1
2	CU	R	192	1/1	0.84	0.16	2.23	78,78,78,78	1
2	CU	T	181	1/1	0.95	0.17	2.20	64,64,64,64	1
2	CU	J	182	1/1	0.94	0.15	1.85	62,62,62,62	1
2	CU	F	181	1/1	0.96	0.17	1.49	74,74,74,74	1
2	CU	B	182	1/1	0.98	0.18	1.48	63,63,63,63	1
2	CU	T	182	1/1	0.97	0.16	1.36	58,58,58,58	1
2	CU	H	182	1/1	0.95	0.15	1.07	54,54,54,54	1
2	CU	J	181	1/1	0.96	0.18	0.86	58,58,58,58	1
2	CU	X	182	1/1	0.96	0.14	0.84	62,62,62,62	1
2	CU	C	181	1/1	0.97	0.12	0.55	80,80,80,80	1
2	CU	Q	182	1/1	0.92	0.13	0.51	67,67,67,67	1
2	CU	V	181	1/1	0.91	0.15	0.39	66,66,66,66	1
2	CU	U	192	1/1	0.91	0.12	0.38	72,72,72,72	1
2	CU	H	181	1/1	0.98	0.13	0.28	65,65,65,65	1
2	CU	E	192	1/1	0.60	0.11	-0.03	71,71,71,71	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CU	U	182	1/1	0.97	0.12	-0.19	68,68,68,68	1
2	CU	C	191	1/1	0.96	0.09	-0.92	61,61,61,61	1
2	CU	L	181	1/1	0.96	0.11	-1.01	61,61,61,61	1
2	CU	G	181	1/1	0.89	0.11	-1.07	67,67,67,67	1
2	CU	E	182	1/1	0.95	0.10	-1.09	66,66,66,66	1
2	CU	L	192	1/1	0.89	0.09	-1.25	73,73,73,73	1
2	CU	J	177	1/1	0.94	0.09	-1.32	65,65,65,65	1
2	CU	N	182	1/1	0.96	0.11	-1.38	62,62,62,62	1
2	CU	J	191	1/1	0.98	0.10	-1.43	52,52,52,52	1
2	CU	H	192	1/1	0.94	0.08	-1.49	69,69,69,69	1
2	CU	O	182	1/1	0.81	0.11	-1.49	63,63,63,63	1
2	CU	B	181	1/1	0.98	0.11	-1.51	67,67,67,67	1
2	CU	X	181	1/1	0.96	0.08	-1.59	55,55,55,55	1
2	CU	D	181	1/1	0.92	0.10	-1.62	65,65,65,65	1
2	CU	A	191	1/1	0.94	0.07	-1.66	41,41,41,41	1
2	CU	A	192	1/1	0.98	0.07	-1.68	58,58,58,58	1
2	CU	K	192	1/1	0.93	0.07	-1.74	56,56,56,56	1
2	CU	I	182	1/1	0.95	0.10	-1.80	57,57,57,57	1
2	CU	F	182	1/1	0.95	0.12	-1.83	56,56,56,56	1
2	CU	D	178	1/1	0.96	0.06	-1.88	61,61,61,61	1
2	CU	N	191	1/1	0.96	0.07	-1.89	46,46,46,46	1
2	CU	I	192	1/1	0.94	0.07	-2.00	64,64,64,64	1
2	CU	B	177	1/1	0.92	0.06	-2.02	70,70,70,70	1
2	CU	T	191	1/1	0.94	0.07	-2.07	69,69,69,69	1
2	CU	D	182	1/1	0.97	0.09	-2.17	64,64,64,64	1
2	CU	A	182	1/1	0.97	0.07	-2.25	65,65,65,65	1
2	CU	S	192	1/1	0.89	0.08	-2.26	74,74,74,74	1
2	CU	S	182	1/1	0.98	0.08	-2.28	62,62,62,62	1
2	CU	W	191	1/1	0.98	0.06	-2.37	56,56,56,56	1
2	CU	W	181	1/1	0.98	0.07	-2.37	61,61,61,61	1
2	CU	G	192	1/1	0.92	0.06	-2.41	61,61,61,61	1
2	CU	G	182	1/1	0.98	0.10	-2.44	67,67,67,67	1
2	CU	L	191	1/1	0.98	0.04	-2.46	62,62,62,62	1
2	CU	V	182	1/1	0.96	0.10	-2.57	62,62,62,62	1
2	CU	A	181	1/1	0.96	0.08	-2.58	65,65,65,65	1
2	CU	L	182	1/1	0.81	0.10	-2.68	51,51,51,51	1
2	CU	F	191	1/1	0.97	0.07	-2.69	53,53,53,53	1
2	CU	V	191	1/1	0.98	0.04	-2.86	56,56,56,56	1
2	CU	S	181	1/1	0.96	0.07	-2.87	71,71,71,71	1
2	CU	R	181	1/1	0.94	0.06	-2.90	60,60,60,60	1
2	CU	M	192	1/1	0.97	0.04	-2.91	69,69,69,69	1
2	CU	K	181	1/1	0.96	0.09	-2.98	65,65,65,65	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CU	S	191	1/1	0.96	0.05	-3.01	66,66,66,66	1
2	CU	B	192	1/1	0.97	0.04	-3.05	64,64,64,64	1
2	CU	N	181	1/1	0.97	0.06	-3.08	63,63,63,63	1
2	CU	R	182	1/1	0.93	0.07	-3.11	55,55,55,55	1
2	CU	O	192	1/1	0.97	0.07	-3.16	59,59,59,59	1
2	CU	N	192	1/1	0.93	0.06	-3.17	67,67,67,67	1
2	CU	D	192	1/1	0.97	0.04	-3.32	56,56,56,56	1
2	CU	W	182	1/1	0.96	0.07	-3.33	53,53,53,53	1
2	CU	D	191	1/1	0.98	0.04	-3.34	61,61,61,61	1
2	CU	K	191	1/1	0.96	0.03	-3.37	46,46,46,46	1
2	CU	E	185	1/1	0.90	0.08	-3.38	49,49,49,49	1
2	CU	G	177	1/1	0.92	0.06	-3.45	62,62,62,62	1
2	CU	J	192	1/1	0.96	0.05	-3.46	60,60,60,60	1
2	CU	P	191	1/1	0.96	0.03	-3.48	53,53,53,53	1
2	CU	X	191	1/1	0.98	0.02	-3.58	51,51,51,51	1
2	CU	K	182	1/1	0.94	0.08	-3.68	54,54,54,54	1
2	CU	E	191	1/1	0.96	0.05	-3.68	58,58,58,58	1
2	CU	G	191	1/1	0.97	0.04	-4.09	55,55,55,55	1
2	CU	U	191	1/1	0.98	0.04	-4.13	46,46,46,46	1
2	CU	O	181	1/1	0.93	0.06	-4.14	59,59,59,59	1
2	CU	C	182	1/1	0.96	0.07	-4.19	53,53,53,53	1
2	CU	E	181	1/1	0.96	0.06	-4.40	65,65,65,65	1
2	CU	P	182	1/1	0.95	0.07	-4.79	60,60,60,60	1
2	CU	C	192	1/1	0.98	0.04	-4.89	57,57,57,57	1
2	CU	M	177	1/1	0.96	0.05	-5.16	58,58,58,58	1
2	CU	M	181	1/1	0.92	0.06	-5.39	54,54,54,54	1
2	CU	O	191	1/1	0.97	0.04	-6.69	52,52,52,52	1
2	CU	H	191	1/1	0.98	0.04	-6.81	49,49,49,49	1
2	CU	Q	181	1/1	0.95	0.05	-7.39	59,59,59,59	1
2	CU	U	181	1/1	0.98	0.07	-10.70	66,66,66,66	1
2	CU	U	185	1/1	0.94	0.05	-	50,50,50,50	1
2	CU	Q	185	1/1	0.91	0.10	-	60,60,60,60	1
2	CU	I	185	1/1	0.85	0.14	-	62,62,62,62	1
2	CU	H	184	1/1	0.90	0.12	-	62,62,62,62	1
2	CU	X	183	1/1	0.97	0.18	-	54,54,54,54	1
2	CU	D	185	1/1	0.95	0.19	-	71,71,71,71	1
2	CU	M	185	1/1	0.72	0.10	-	62,62,62,62	1
2	CU	G	185	1/1	0.89	0.16	-	55,55,55,55	1
2	CU	Q	183	1/1	0.94	0.14	-	54,54,54,54	1
2	CU	A	190	1/1	0.99	0.04	-	37,37,37,37	1
2	CU	L	184	1/1	0.90	0.11	-	62,62,62,62	1
2	CU	E	184	1/1	0.81	0.10	-	59,59,59,59	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CU	B	190	1/1	0.97	0.04	-	34,34,34,34	1
2	CU	R	184	1/1	0.92	0.19	-	64,64,64,64	1
2	CU	R	183	1/1	0.97	0.13	-	58,58,58,58	1
2	CU	P	184	1/1	0.75	0.13	-	63,63,63,63	1
2	CU	X	185	1/1	0.82	0.11	-	54,54,54,54	1
2	CU	W	183	1/1	0.96	0.13	-	61,61,61,61	1
2	CU	D	184	1/1	0.90	0.15	-	65,65,65,65	1
2	CU	I	191	1/1	0.98	0.05	-	56,56,56,56	1
2	CU	P	185	1/1	0.75	0.12	-	57,57,57,57	1
2	CU	W	185	1/1	0.92	0.18	-	56,56,56,56	1
2	CU	J	185	1/1	0.94	0.08	-	55,55,55,55	1
2	CU	A	184	1/1	0.93	0.12	-	57,57,57,57	1
2	CU	S	183	1/1	0.96	0.07	-	59,59,59,59	1
2	CU	X	184	1/1	0.78	0.11	-	58,58,58,58	1
2	CU	P	183	1/1	0.93	0.20	-	61,61,61,61	1
2	CU	N	183	1/1	0.92	0.17	-	63,63,63,63	1
2	CU	M	191	1/1	0.92	0.09	-	67,67,67,67	1
2	CU	J	184	1/1	0.90	0.08	-	55,55,55,55	1
2	CU	B	191	1/1	0.99	0.02	-	52,52,52,52	1
2	CU	D	183	1/1	0.91	0.13	-	66,66,66,66	1
2	CU	Q	191	1/1	0.98	0.04	-	46,46,46,46	1
2	CU	F	183	1/1	0.95	0.31	-	58,58,58,58	1
2	CU	L	185	1/1	0.90	0.16	-	62,62,62,62	1
2	CU	A	183	1/1	0.97	0.11	-	61,61,61,61	1
2	CU	B	184	1/1	0.68	0.15	-	75,75,75,75	1
2	CU	R	185	1/1	0.74	0.14	-	57,57,57,57	1
2	CU	C	185	1/1	0.88	0.15	-	59,59,59,59	1
2	CU	O	185	1/1	0.93	0.14	-	53,53,53,53	1
2	CU	C	184	1/1	0.94	0.12	-	59,59,59,59	1
2	CU	B	183	1/1	0.98	0.17	-	56,56,56,56	1
2	CU	C	183	1/1	0.95	0.14	-	60,60,60,60	1
2	CU	L	183	1/1	0.90	0.11	-	63,63,63,63	1
2	CU	H	183	1/1	0.96	0.18	-	52,52,52,52	1
2	CU	A	185	1/1	0.84	0.13	-	58,58,58,58	1
2	CU	J	183	1/1	0.96	0.19	-	57,57,57,57	1
2	CU	N	184	1/1	0.89	0.11	-	55,55,55,55	1
2	CU	D	177	1/1	0.94	0.08	-	64,64,64,64	1
2	CU	D	190	1/1	0.99	0.03	-	32,32,32,32	1
2	CU	T	183	1/1	0.94	0.23	-	57,57,57,57	1
2	CU	Q	184	1/1	0.83	0.14	-	57,57,57,57	1
2	CU	I	181	1/1	0.97	0.07	-	50,50,50,50	1
2	CU	U	183	1/1	0.95	0.07	-	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CU	M	183	1/1	0.94	0.10	-	61,61,61,61	1
2	CU	E	190	1/1	1.00	0.02	-	34,34,34,34	1
2	CU	F	184	1/1	0.64	0.14	-	57,57,57,57	1
2	CU	R	191	1/1	0.96	0.04	-	45,45,45,45	1
2	CU	F	190	1/1	0.98	0.04	-	33,33,33,33	1
2	CU	K	177	1/1	0.93	0.09	-	66,66,66,66	1
2	CU	V	183	1/1	0.89	0.14	-	56,56,56,56	1
2	CU	K	185	1/1	0.94	0.06	-	55,55,55,55	1
2	CU	N	190	1/1	1.00	0.02	-	32,32,32,32	1
2	CU	V	185	1/1	0.91	0.08	-	61,61,61,61	1
2	CU	M	184	1/1	0.93	0.11	-	56,56,56,56	1
2	CU	I	184	1/1	0.79	0.09	-	59,59,59,59	1
2	CU	G	184	1/1	0.91	0.12	-	64,64,64,64	1
2	CU	O	183	1/1	0.97	0.06	-	59,59,59,59	1
2	CU	E	183	1/1	0.94	0.13	-	61,61,61,61	1
2	CU	I	183	1/1	0.91	0.13	-	60,60,60,60	1
2	CU	G	183	1/1	0.97	0.09	-	53,53,53,53	1
2	CU	W	184	1/1	0.84	0.19	-	66,66,66,66	1

6.5 Other polymers (i)

There are no such residues in this entry.