



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:04 AM UTC

PDB ID : 1OZT / pdb_00001ozt
Title : Crystal Structure of apo-H46R Familial ALS Mutant human Cu,Zn Superoxide Dismutase (CuZnSOD) to 2.5Å resolution
Authors : Elam, J.S.; Taylor, A.B.; Strange, R.; Antonyuk, S.; Doucette, P.A.; Rodriguez, J.A.; Hasnain, S.S.; Hayward, L.J.; Valentine, J.S.; Yeates, T.O.; Hart, P.J.
Deposited on : 2003-04-09
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

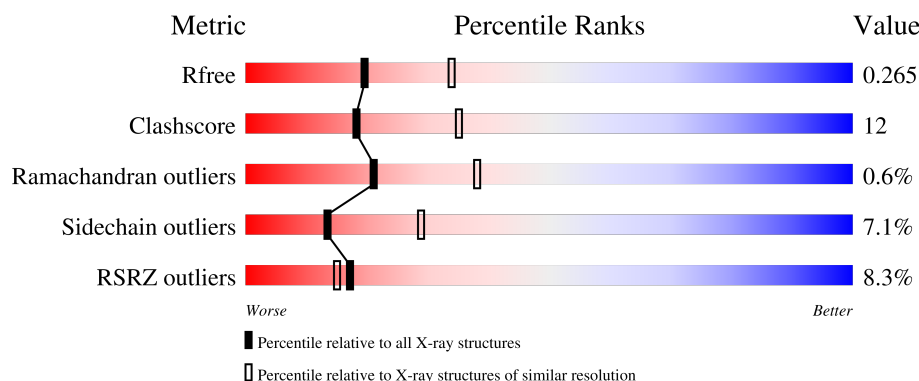
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	G	153	9% 65% 17% • 15%
1	H	153	6% 65% 21% • 12%
1	I	153	6% 63% 20% 6% 12%
1	J	153	14% 66% 16% 6% • 12%
1	K	153	5% 61% 18% • 18%

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Mol	Chain	Length	Quality of chain
1	L	153	6% 63% 18% • 15%
1	M	153	9% 69% 25% 5%
1	N	153	5% 74% 21% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8201 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	153	Total	C	N	O	S	0	0	0
			1111	679	204	224	4			
1	N	153	Total	C	N	O	S	0	0	0
			1111	679	204	224	4			
1	G	130	Total	C	N	O	S	0	0	0
			945	584	170	187	4			
1	H	135	Total	C	N	O	S	0	0	0
			975	601	177	193	4			
1	K	126	Total	C	N	O	S	0	0	0
			921	570	166	181	4			
1	L	130	Total	C	N	O	S	0	0	0
			941	580	171	186	4			
1	I	135	Total	C	N	O	S	0	0	0
			979	603	177	195	4			
1	J	135	Total	C	N	O	S	0	0	0
			983	605	180	194	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	46	ARG	HIS	engineered mutation	UNP P00441
N	46	ARG	HIS	engineered mutation	UNP P00441
G	46	ARG	HIS	engineered mutation	UNP P00441
H	46	ARG	HIS	engineered mutation	UNP P00441
K	46	ARG	HIS	engineered mutation	UNP P00441
L	46	ARG	HIS	engineered mutation	UNP P00441
I	46	ARG	HIS	engineered mutation	UNP P00441
J	46	ARG	HIS	engineered mutation	UNP P00441

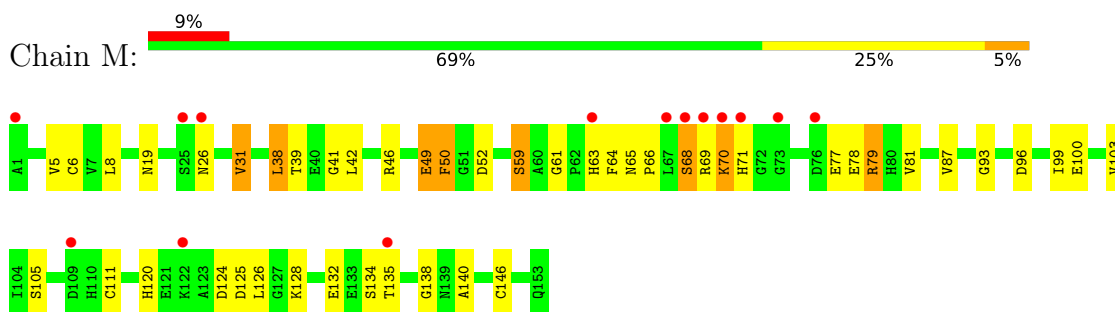
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	M	25	Total 25	O 25	0	0
2	N	48	Total 48	O 48	0	0
2	G	23	Total 23	O 23	0	0
2	H	30	Total 30	O 30	0	0
2	K	32	Total 32	O 32	0	0
2	L	40	Total 40	O 40	0	0
2	I	22	Total 22	O 22	0	0
2	J	15	Total 15	O 15	0	0

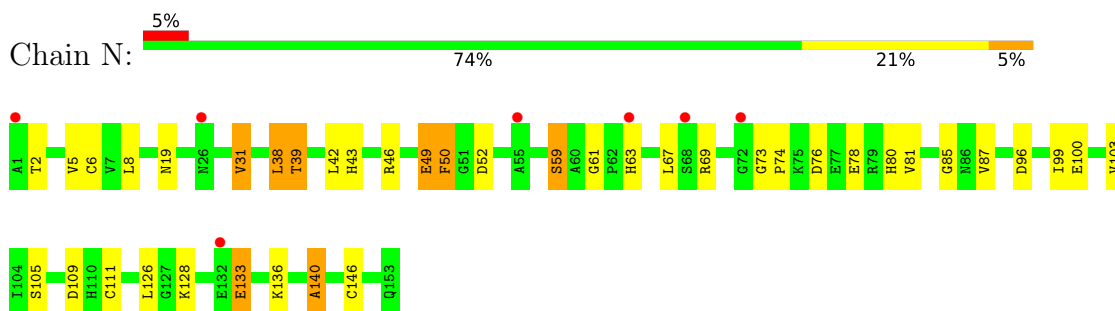
3 Residue-property plots [i](#)

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.

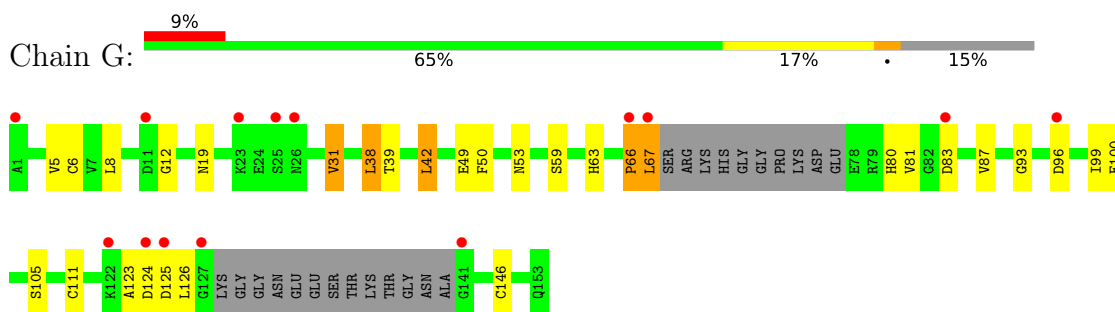
- Molecule 1: Superoxide dismutase [Cu-Zn]



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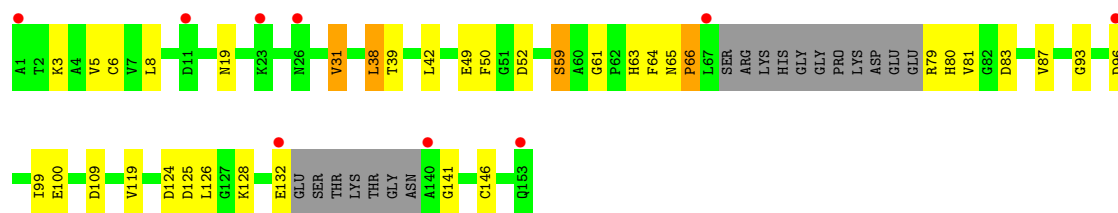


- Molecule 1: Superoxide dismutase [Cu-Zn]

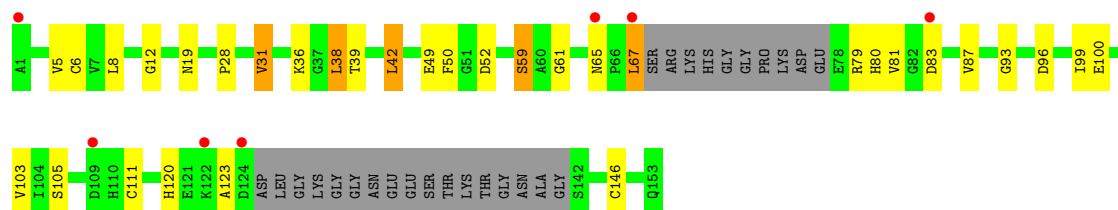


- Molecule 1: Superoxide dismutase [Cu-Zn]

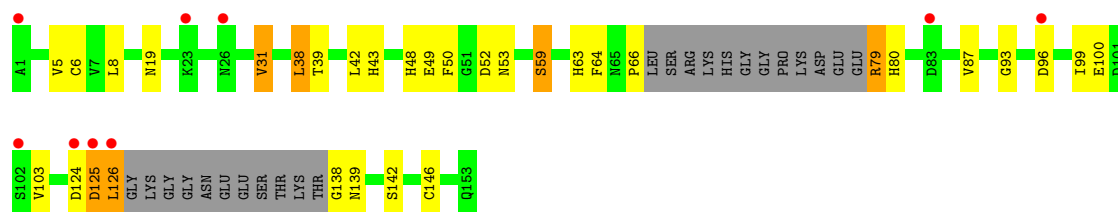




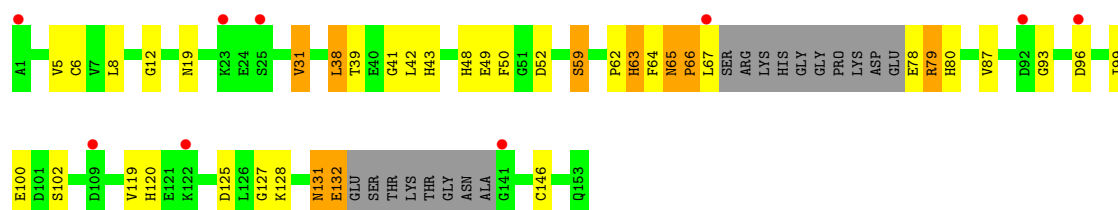
• Molecule 1: Superoxide dismutase [Cu-Zn]



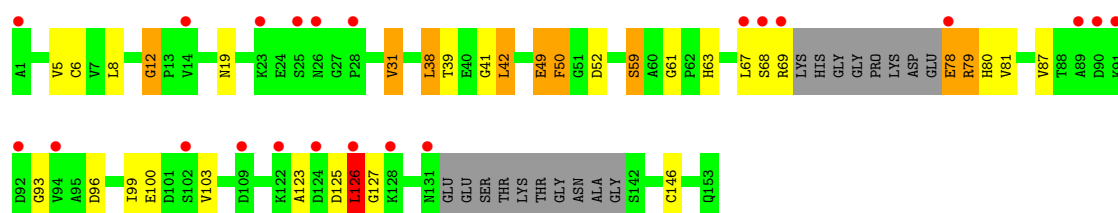
• Molecule 1: Superoxide dismutase [Cu-Zn]



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.62Å 70.00Å 113.79Å 90.00° 110.37° 90.00°	Depositor
Resolution (Å)	42.43 – 2.50 42.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.43-2.50) 99.7 (42.43-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.270 0.218 , 0.265	Depositor DCC
R_{free} test set	1988 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8201	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	G	0.70	0/958	1.14	7/1291 (0.5%)
1	H	0.70	0/988	1.19	8/1330 (0.6%)
1	I	0.67	0/992	1.18	10/1335 (0.7%)
1	J	0.63	0/996	1.13	10/1340 (0.7%)
1	K	0.70	0/934	1.16	10/1259 (0.8%)
1	L	0.78	0/954	1.11	4/1286 (0.3%)
1	M	0.71	0/1128	1.21	10/1519 (0.7%)
1	N	0.76	0/1128	1.20	8/1519 (0.5%)
All	All	0.71	0/8078	1.17	67/10879 (0.6%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	ASN	CA-C-N	10.99	133.58	119.84
1	I	65	ASN	C-N-CA	10.99	133.58	119.84
1	M	126	LEU	N-CA-C	-10.04	100.97	113.23
1	M	61	GLY	CA-C-N	10.01	129.82	120.21
1	M	61	GLY	C-N-CA	10.01	129.82	120.21
1	N	61	GLY	CA-C-N	9.42	129.25	120.21
1	N	61	GLY	C-N-CA	9.42	129.25	120.21
1	J	61	GLY	CA-C-N	8.77	128.63	120.21
1	J	61	GLY	C-N-CA	8.77	128.63	120.21
1	H	65	ASN	CA-C-N	8.31	130.23	119.84
1	H	65	ASN	C-N-CA	8.31	130.23	119.84
1	M	49	GLU	N-CA-C	8.01	121.03	111.33
1	I	49	GLU	N-CA-C	7.87	120.86	111.33
1	G	124	ASP	N-CA-C	-7.77	96.60	108.96
1	J	49	GLU	N-CA-C	7.55	120.47	111.33
1	K	49	GLU	N-CA-C	7.49	120.10	111.11
1	H	49	GLU	N-CA-C	7.49	120.39	111.33
1	G	49	GLU	N-CA-C	7.43	120.32	111.33
1	N	49	GLU	N-CA-C	7.41	120.30	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	87	VAL	N-CA-C	-7.30	97.61	108.85
1	H	61	GLY	CA-C-N	7.29	128.95	119.84
1	H	61	GLY	C-N-CA	7.29	128.95	119.84
1	L	49	GLU	N-CA-C	6.91	118.81	111.28
1	N	87	VAL	N-CA-C	-6.78	98.41	108.85
1	K	65	ASN	CA-C-N	6.77	128.30	119.84
1	K	65	ASN	C-N-CA	6.77	128.30	119.84
1	G	87	VAL	N-CA-C	-6.70	98.54	108.85
1	M	65	ASN	CA-C-N	6.66	127.20	119.47
1	M	65	ASN	C-N-CA	6.66	127.20	119.47
1	L	39	THR	N-CA-C	-6.59	100.72	110.48
1	M	77	GLU	N-CA-C	-6.52	103.38	112.45
1	N	50	PHE	N-CA-C	6.46	120.00	109.59
1	L	50	PHE	N-CA-C	6.43	119.94	109.59
1	J	87	VAL	N-CA-C	-6.22	99.27	108.85
1	K	50	PHE	N-CA-C	6.02	119.28	109.59
1	N	67	LEU	N-CA-C	5.94	120.13	112.41
1	J	50	PHE	N-CA-C	5.93	119.13	109.59
1	K	87	VAL	N-CA-C	-5.88	99.80	108.85
1	H	87	VAL	N-CA-C	-5.81	99.90	108.85
1	G	50	PHE	N-CA-C	5.72	118.79	109.59
1	N	140	ALA	N-CA-C	5.71	119.98	112.89
1	K	61	GLY	CA-C-N	5.60	126.06	120.52
1	K	61	GLY	C-N-CA	5.60	126.06	120.52
1	N	39	THR	N-CA-C	-5.60	102.20	110.48
1	L	87	VAL	N-CA-C	-5.59	100.25	108.85
1	J	41	GLY	N-CA-C	5.47	118.69	111.52
1	I	12	GLY	CA-C-N	5.44	126.29	120.47
1	I	12	GLY	C-N-CA	5.44	126.29	120.47
1	G	39	THR	N-CA-C	-5.37	102.54	110.48
1	I	39	THR	N-CA-C	-5.36	102.55	110.48
1	K	12	GLY	CA-C-N	5.30	127.30	120.89
1	K	12	GLY	C-N-CA	5.30	127.30	120.89
1	I	120	HIS	N-CA-C	5.29	118.73	110.32
1	I	50	PHE	N-CA-C	5.28	118.09	109.59
1	G	12	GLY	CA-C-N	5.27	126.11	120.47
1	G	12	GLY	C-N-CA	5.27	126.11	120.47
1	K	120	HIS	N-CA-C	5.27	118.58	110.42
1	I	41	GLY	N-CA-C	5.26	118.44	110.97
1	I	87	VAL	N-CA-C	-5.26	100.75	108.85
1	H	50	PHE	N-CA-C	5.22	117.99	109.59
1	J	68	SER	N-CA-C	5.15	121.76	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	J	39	THR	N-CA-C	-5.15	102.86	110.48
1	M	41	GLY	N-CA-C	5.14	118.25	111.52
1	J	12	GLY	CA-C-N	5.13	125.96	120.47
1	J	12	GLY	C-N-CA	5.13	125.96	120.47
1	H	39	THR	N-CA-C	-5.05	103.00	110.48
1	M	50	PHE	N-CA-C	5.03	117.68	109.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	945	0	924	22	0
1	H	975	0	954	19	0
1	I	979	0	955	23	0
1	J	983	0	964	23	0
1	K	921	0	903	18	0
1	L	941	0	918	29	0
1	M	1111	0	1083	32	0
1	N	1111	0	1083	32	0
2	G	23	0	0	1	0
2	H	30	0	0	2	0
2	I	22	0	0	1	0
2	J	15	0	0	2	0
2	K	32	0	0	4	0
2	L	40	0	0	4	0
2	M	25	0	0	2	0
2	N	48	0	0	4	0
All	All	8201	0	7784	191	0

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

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:26:ASN:HD22	1:G:67:LEU:HD21	1.28	0.99
1:J:78:GLU:HG3	1:J:79:ARG:N	1.85	0.90
1:J:78:GLU:HG3	1:J:79:ARG:H	1.38	0.88
1:G:66:PRO:O	1:G:67:LEU:HD13	1.75	0.87
1:G:66:PRO:C	1:G:67:LEU:HD22	2.00	0.87
1:J:126:LEU:HD12	1:J:126:LEU:H	1.38	0.86
1:M:70:LYS:HE2	1:M:70:LYS:H	1.41	0.85
1:J:81:VAL:HG23	2:J:156:HOH:O	1.78	0.84
1:M:26:ASN:ND2	1:G:67:LEU:HD21	1.91	0.83
1:L:125:ASP:HB2	1:L:126:LEU:HD23	1.59	0.83
1:N:69:ARG:CD	1:N:78:GLU:HG3	2.10	0.81
1:M:70:LYS:HE2	1:M:70:LYS:N	1.95	0.80
1:J:126:LEU:HD12	1:J:126:LEU:N	2.01	0.75
1:M:26:ASN:HB2	1:G:67:LEU:HD23	1.67	0.74
1:N:69:ARG:HD3	1:N:78:GLU:HG3	1.71	0.71
1:L:126:LEU:HG	1:L:138:GLY:CA	2.21	0.71
1:N:126:LEU:HB2	1:N:128:LYS:HE3	1.72	0.71
1:J:78:GLU:CG	1:J:79:ARG:N	2.55	0.70
1:N:69:ARG:HB3	1:N:78:GLU:CG	2.23	0.68
1:N:69:ARG:HD2	1:N:78:GLU:HG3	1.77	0.67
1:H:141:GLY:HA3	2:H:161:HOH:O	1.95	0.67
1:I:66:PRO:O	1:I:67:LEU:HB2	1.93	0.67
1:N:46:ARG:HH22	1:N:140:ALA:HB2	1.60	0.66
1:L:64:PHE:CZ	1:L:66:PRO:HG3	2.30	0.66
1:G:67:LEU:HD22	1:G:67:LEU:N	2.11	0.66
1:L:126:LEU:HG	1:L:138:GLY:N	2.11	0.66
1:J:126:LEU:H	1:J:126:LEU:CD1	2.09	0.65
1:L:126:LEU:HG	1:L:138:GLY:HA2	1.76	0.65
1:L:142:SER:HB2	2:L:177:HOH:O	1.96	0.65
1:I:132:GLU:OE1	1:I:132:GLU:HA	1.97	0.64
1:M:8:LEU:HD12	1:M:146:CYS:HA	1.80	0.63
1:M:26:ASN:HD22	1:G:67:LEU:CD2	2.08	0.63
1:M:39:THR:HG23	2:M:168:HOH:O	1.98	0.62
1:M:64:PHE:CZ	1:M:66:PRO:HG3	2.33	0.62
1:N:73:GLY:H	1:N:76:ASP:HB2	1.64	0.62
1:M:26:ASN:HB2	1:G:67:LEU:CD2	2.30	0.61
1:I:63:HIS:CE1	1:I:80:HIS:CD2	2.88	0.61
1:M:125:ASP:HB2	1:M:138:GLY:HA2	1.82	0.61
1:K:8:LEU:HD12	1:K:146:CYS:HA	1.83	0.61
1:I:8:LEU:HD12	1:I:146:CYS:HA	1.81	0.60
1:N:133:GLU:HA	1:N:133:GLU:OE1	2.01	0.60
1:H:125:ASP:O	1:H:126:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:HIS:HD2	1:L:63:HIS:O	1.85	0.59
1:J:79:ARG:HG3	1:J:80:HIS:N	2.15	0.59
1:K:67:LEU:HB3	2:K:179:HOH:O	2.03	0.58
1:L:126:LEU:HD21	2:L:184:HOH:O	2.03	0.57
1:N:2:THR:HG21	2:N:187:HOH:O	2.04	0.57
1:L:8:LEU:HD12	1:L:146:CYS:HA	1.85	0.57
1:G:66:PRO:HD2	1:G:81:VAL:HG21	1.88	0.56
1:H:8:LEU:HD12	1:H:146:CYS:HA	1.87	0.56
1:N:8:LEU:HD12	1:N:146:CYS:HA	1.87	0.55
1:N:69:ARG:HB3	1:N:78:GLU:HG3	1.88	0.55
1:G:80:HIS:HB2	1:G:83:ASP:OD2	2.07	0.55
1:N:69:ARG:HB3	1:N:78:GLU:HG2	1.89	0.55
1:H:63:HIS:NE2	1:H:80:HIS:ND1	2.54	0.54
1:J:99:ILE:HG22	1:J:100:GLU:N	2.22	0.54
1:L:126:LEU:CG	1:L:138:GLY:N	2.71	0.54
1:M:132:GLU:HA	1:M:132:GLU:OE1	2.07	0.53
1:G:8:LEU:HD12	1:G:146:CYS:HA	1.88	0.53
1:I:66:PRO:O	1:I:67:LEU:CB	2.56	0.53
1:I:79:ARG:O	1:I:79:ARG:HG3	2.08	0.53
1:I:65:ASN:ND2	1:I:80:HIS:CD2	2.77	0.53
1:L:63:HIS:CE1	1:L:80:HIS:HD1	2.27	0.52
1:N:74:PRO:HG3	1:N:85:GLY:N	2.25	0.52
1:J:8:LEU:HD12	1:J:146:CYS:HA	1.91	0.52
1:J:52:ASP:O	1:J:59:SER:HB2	2.09	0.52
1:M:64:PHE:CE1	1:M:66:PRO:HG3	2.45	0.52
1:I:5:VAL:HG22	1:I:6:CYS:N	2.23	0.52
1:N:46:ARG:NH2	1:N:140:ALA:HB2	2.25	0.52
1:J:5:VAL:HG22	1:J:6:CYS:N	2.24	0.52
1:L:63:HIS:NE2	1:L:80:HIS:ND1	2.52	0.51
1:M:105:SER:O	1:M:111:CYS:HA	2.11	0.51
1:J:125:ASP:C	1:J:127:GLY:H	2.18	0.51
1:K:79:ARG:HG2	1:K:80:HIS:N	2.25	0.51
1:M:46:ARG:HD2	1:M:63:HIS:NE2	2.26	0.51
1:N:46:ARG:HG2	2:N:169:HOH:O	2.11	0.50
1:L:139:ASN:HB3	2:L:167:HOH:O	2.12	0.50
1:J:67:LEU:HD13	2:J:163:HOH:O	2.12	0.50
1:G:99:ILE:HG22	1:G:100:GLU:N	2.26	0.50
1:H:5:VAL:HG22	1:H:6:CYS:N	2.27	0.50
1:K:99:ILE:HG22	1:K:100:GLU:N	2.26	0.50
1:L:125:ASP:HB2	1:L:126:LEU:CD2	2.36	0.50
1:N:52:ASP:O	1:N:59:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:VAL:HG22	1:K:6:CYS:N	2.27	0.49
1:K:39:THR:HG22	1:J:12:GLY:HA2	1.93	0.49
1:L:48:HIS:HA	1:L:63:HIS:HA	1.94	0.49
1:J:19:ASN:O	1:J:31:VAL:HA	2.13	0.49
1:H:99:ILE:HG22	1:H:100:GLU:N	2.27	0.49
1:L:99:ILE:HG22	1:L:100:GLU:N	2.28	0.49
1:G:125:ASP:O	1:G:126:LEU:HB2	2.13	0.49
1:L:79:ARG:NH2	1:L:103:VAL:HB	2.28	0.49
1:N:99:ILE:HG22	1:N:100:GLU:N	2.27	0.48
1:L:63:HIS:O	1:L:63:HIS:CD2	2.64	0.48
1:I:19:ASN:O	1:I:31:VAL:HA	2.13	0.48
1:M:99:ILE:HG22	1:M:100:GLU:N	2.27	0.48
1:I:125:ASP:OD1	1:I:127:GLY:N	2.40	0.48
1:L:19:ASN:O	1:L:31:VAL:HA	2.14	0.48
1:M:120:HIS:CB	1:M:140:ALA:HB1	2.44	0.47
1:K:52:ASP:O	1:K:59:SER:HB2	2.14	0.47
1:I:48:HIS:HA	1:I:63:HIS:HA	1.96	0.47
1:J:38:LEU:O	1:J:93:GLY:HA2	2.14	0.47
1:L:38:LEU:HG	1:L:43:HIS:CD2	2.48	0.47
1:H:79:ARG:NH2	1:H:83:ASP:O	2.47	0.47
1:M:46:ARG:HH21	1:M:124:ASP:CG	2.22	0.47
1:M:5:VAL:HG22	1:M:6:CYS:N	2.30	0.47
1:M:71:HIS:HB3	1:M:135:THR:O	2.14	0.47
1:K:38:LEU:O	1:K:93:GLY:HA2	2.15	0.47
1:M:19:ASN:O	1:M:31:VAL:HA	2.15	0.47
1:H:52:ASP:O	1:H:59:SER:HB2	2.15	0.47
1:K:36:LYS:HB2	2:K:160:HOH:O	2.15	0.46
1:L:53:ASN:HB2	2:L:191:HOH:O	2.14	0.46
1:J:63:HIS:CE1	1:J:80:HIS:ND1	2.84	0.46
1:N:19:ASN:O	1:N:31:VAL:HA	2.15	0.46
1:N:74:PRO:HG2	1:N:85:GLY:HA3	1.97	0.46
1:M:46:ARG:HH22	1:M:140:ALA:HB2	1.80	0.46
1:H:19:ASN:O	1:H:31:VAL:HA	2.15	0.46
1:L:52:ASP:O	1:L:59:SER:HB2	2.15	0.46
1:L:126:LEU:HD23	1:L:126:LEU:N	2.30	0.46
1:J:99:ILE:CG2	1:J:100:GLU:N	2.78	0.46
1:M:38:LEU:O	1:M:93:GLY:HA2	2.15	0.46
1:K:28:PRO:HD2	2:K:185:HOH:O	2.15	0.46
1:L:63:HIS:HE2	1:L:80:HIS:HD1	1.59	0.46
1:G:5:VAL:HG22	1:G:6:CYS:N	2.31	0.46
1:K:19:ASN:O	1:K:31:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:VAL:HG22	1:N:6:CYS:N	2.30	0.45
1:I:99:ILE:HG22	1:I:100:GLU:N	2.30	0.45
1:I:52:ASP:O	1:I:59:SER:HB2	2.16	0.45
1:N:2:THR:CG2	2:N:187:HOH:O	2.62	0.45
1:G:63:HIS:CE1	1:G:80:HIS:HD1	2.35	0.45
1:J:49:GLU:HG2	1:J:50:PHE:CE1	2.52	0.44
1:L:38:LEU:O	1:L:93:GLY:HA2	2.18	0.44
1:I:64:PHE:CZ	1:I:66:PRO:HG3	2.52	0.44
1:M:66:PRO:HG2	1:M:81:VAL:HG21	1.98	0.44
1:M:128:LYS:HE2	2:M:164:HOH:O	2.18	0.44
1:G:67:LEU:N	1:G:67:LEU:CD2	2.81	0.44
1:K:67:LEU:C	2:K:179:HOH:O	2.61	0.44
1:K:81:VAL:HG13	1:K:103:VAL:HG12	1.99	0.44
1:N:99:ILE:CG2	1:N:100:GLU:N	2.81	0.43
1:H:99:ILE:CG2	1:H:100:GLU:N	2.82	0.43
1:N:38:LEU:HG	1:N:43:HIS:CD2	2.53	0.43
1:N:74:PRO:CG	1:N:85:GLY:HA3	2.48	0.43
1:L:5:VAL:HG22	1:L:6:CYS:N	2.32	0.43
1:I:65:ASN:HA	1:I:66:PRO:HD3	1.75	0.43
1:H:80:HIS:N	1:H:80:HIS:CD2	2.86	0.43
1:M:69:ARG:HD3	1:M:78:GLU:OE1	2.18	0.43
1:I:131:ASN:HB2	1:I:132:GLU:H	1.51	0.43
1:I:119:VAL:O	1:I:119:VAL:HG13	2.19	0.43
1:K:105:SER:O	1:K:111:CYS:HA	2.19	0.43
1:H:3:LYS:HD2	2:H:164:HOH:O	2.17	0.43
1:H:38:LEU:O	1:H:93:GLY:HA2	2.18	0.43
1:I:102:SER:HB2	2:I:175:HOH:O	2.18	0.43
1:H:119:VAL:O	1:H:119:VAL:HG13	2.19	0.42
1:M:79:ARG:NH2	1:M:103:VAL:HB	2.34	0.42
1:N:133:GLU:OE1	1:N:136:LYS:HD2	2.18	0.42
1:I:38:LEU:O	1:I:93:GLY:HA2	2.19	0.42
1:N:63:HIS:ND1	1:N:80:HIS:ND1	2.64	0.42
1:H:66:PRO:HD2	1:H:81:VAL:HG21	2.02	0.42
1:G:38:LEU:O	1:G:93:GLY:HA2	2.20	0.42
1:H:64:PHE:CE1	1:H:66:PRO:HG3	2.55	0.42
1:K:99:ILE:CG2	1:K:100:GLU:N	2.82	0.42
1:N:49:GLU:HG2	1:N:50:PHE:CE1	2.55	0.42
1:H:124:ASP:OD1	1:H:125:ASP:N	2.52	0.42
1:J:81:VAL:HG13	1:J:103:VAL:HG12	2.01	0.42
1:M:99:ILE:CG2	1:M:100:GLU:N	2.83	0.42
1:J:69:ARG:HA	1:J:69:ARG:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ILE:CG2	1:G:100:GLU:N	2.83	0.41
1:K:42:LEU:HB3	1:K:123:ALA:HB2	2.02	0.41
1:N:46:ARG:HH22	1:N:140:ALA:CB	2.32	0.41
1:L:64:PHE:CE1	1:L:66:PRO:HG3	2.54	0.41
1:N:39:THR:HG23	2:N:198:HOH:O	2.21	0.41
1:N:81:VAL:HG13	1:N:103:VAL:HG12	2.02	0.41
1:I:38:LEU:HG	1:I:43:HIS:CD2	2.55	0.41
1:G:53:ASN:HB2	2:G:170:HOH:O	2.19	0.41
1:N:105:SER:O	1:N:111:CYS:HA	2.20	0.41
1:I:99:ILE:CG2	1:I:100:GLU:N	2.84	0.41
1:J:42:LEU:HB3	1:J:123:ALA:HB2	2.02	0.41
1:G:42:LEU:HB3	1:G:123:ALA:HB2	2.03	0.41
1:L:124:ASP:OD1	1:L:125:ASP:N	2.53	0.41
1:M:66:PRO:HD2	1:M:81:VAL:CG2	2.51	0.41
1:M:125:ASP:OD2	1:M:134:SER:CB	2.69	0.41
1:N:109:ASP:OD2	1:H:109:ASP:HB2	2.21	0.41
1:G:19:ASN:O	1:G:31:VAL:HA	2.21	0.41
1:K:67:LEU:HA	1:K:67:LEU:HD13	1.88	0.41
1:K:80:HIS:HB2	1:K:83:ASP:OD2	2.21	0.41
1:L:99:ILE:CG2	1:L:100:GLU:N	2.84	0.41
1:I:125:ASP:OD1	1:I:125:ASP:C	2.64	0.41
1:G:105:SER:O	1:G:111:CYS:HA	2.21	0.40
1:M:49:GLU:HG2	1:M:50:PHE:CE1	2.57	0.40
1:I:131:ASN:O	1:I:132:GLU:HB2	2.19	0.40
1:M:52:ASP:O	1:M:59:SER:HB2	2.22	0.40
1:H:124:ASP:OD1	1:H:124:ASP:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	124/153 (81%)	118 (95%)	5 (4%)	1 (1%)	16	31
1	H	129/153 (84%)	124 (96%)	4 (3%)	1 (1%)	16	31
1	I	129/153 (84%)	122 (95%)	5 (4%)	2 (2%)	7	14
1	J	129/153 (84%)	122 (95%)	6 (5%)	1 (1%)	16	31
1	K	120/153 (78%)	115 (96%)	5 (4%)	0	100	100
1	L	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
1	M	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	18	34
1	N	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
All	All	1057/1224 (86%)	1007 (95%)	44 (4%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	66	PRO
1	M	68	SER
1	H	66	PRO
1	J	126	LEU
1	I	128	LYS
1	I	66	PRO

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	G	101/118 (86%)	95 (94%)	6 (6%)	18	37
1	H	103/118 (87%)	96 (93%)	7 (7%)	14	31
1	I	104/118 (88%)	93 (89%)	11 (11%)	6	14
1	J	105/118 (89%)	97 (92%)	8 (8%)	12	26
1	K	99/118 (84%)	93 (94%)	6 (6%)	17	35
1	L	100/118 (85%)	92 (92%)	8 (8%)	11	24
1	M	118/118 (100%)	110 (93%)	8 (7%)	14	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	118/118 (100%)	112 (95%)	6 (5%)	21	43
All	All	848/944 (90%)	788 (93%)	60 (7%)	13	29

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	31	VAL
1	M	38	LEU
1	M	42	LEU
1	M	59	SER
1	M	68	SER
1	M	70	LYS
1	M	79	ARG
1	M	96	ASP
1	N	31	VAL
1	N	38	LEU
1	N	42	LEU
1	N	59	SER
1	N	96	ASP
1	N	133	GLU
1	G	31	VAL
1	G	38	LEU
1	G	42	LEU
1	G	59	SER
1	G	67	LEU
1	G	96	ASP
1	H	31	VAL
1	H	38	LEU
1	H	42	LEU
1	H	59	SER
1	H	96	ASP
1	H	128	LYS
1	H	132	GLU
1	K	31	VAL
1	K	38	LEU
1	K	42	LEU
1	K	59	SER
1	K	67	LEU
1	K	96	ASP
1	L	31	VAL
1	L	38	LEU
1	L	42	LEU

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Mol	Chain	Res	Type
1	L	59	SER
1	L	79	ARG
1	L	96	ASP
1	L	125	ASP
1	L	126	LEU
1	I	31	VAL
1	I	38	LEU
1	I	42	LEU
1	I	59	SER
1	I	62	PRO
1	I	63	HIS
1	I	78	GLU
1	I	79	ARG
1	I	96	ASP
1	I	131	ASN
1	I	132	GLU
1	J	31	VAL
1	J	38	LEU
1	J	42	LEU
1	J	59	SER
1	J	78	GLU
1	J	79	ARG
1	J	96	ASP
1	J	126	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	153	GLN
1	N	153	GLN
1	G	153	GLN
1	H	65	ASN
1	H	153	GLN
1	K	153	GLN
1	L	65	ASN
1	L	153	GLN
1	I	63	HIS
1	I	65	ASN
1	I	80	HIS
1	I	153	GLN
1	J	53	ASN
1	J	63	HIS

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Mol	Chain	Res	Type
1	J	153	GLN

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	G	130/153 (84%)	0.48	14 (10%) 11 9	9, 37, 80, 101	0
1	H	135/153 (88%)	0.39	9 (6%) 24 21	18, 38, 75, 100	0
1	I	135/153 (88%)	0.52	9 (6%) 24 21	15, 41, 72, 96	0
1	J	135/153 (88%)	0.83	22 (16%) 4 3	20, 48, 92, 101	0
1	K	126/153 (82%)	0.41	7 (5%) 30 26	18, 36, 72, 95	0
1	L	130/153 (84%)	0.31	9 (6%) 23 20	16, 31, 75, 101	0
1	M	153/153 (100%)	0.61	14 (9%) 14 13	16, 41, 86, 101	0
1	N	153/153 (100%)	0.29	7 (4%) 37 33	9, 34, 81, 101	0
All	All	1097/1224 (89%)	0.48	91 (8%) 17 15	9, 38, 81, 101	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	ALA	4.7
1	L	126	LEU	4.7
1	I	1	ALA	4.5
1	M	67	LEU	4.5
1	N	1	ALA	4.2
1	I	67	LEU	4.1
1	I	141	GLY	3.9
1	M	70	LYS	3.8
1	I	109	ASP	3.8
1	M	68	SER	3.7
1	L	1	ALA	3.7
1	L	26	ASN	3.7
1	G	127	GLY	3.6
1	L	83	ASP	3.6
1	M	1	ALA	3.6
1	J	1	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	26	ASN	3.6
1	J	26	ASN	3.6
1	H	96	ASP	3.4
1	G	141	GLY	3.4
1	K	109	ASP	3.3
1	J	92	ASP	3.3
1	L	96	ASP	3.3
1	K	67	LEU	3.3
1	G	26	ASN	3.2
1	J	23	LYS	3.2
1	M	26	ASN	3.2
1	N	63	HIS	3.2
1	N	68	SER	3.1
1	G	125	ASP	3.1
1	G	1	ALA	3.1
1	M	71	HIS	3.1
1	M	63	HIS	3.0
1	I	122	LYS	3.0
1	H	67	LEU	2.9
1	I	25	SER	2.9
1	H	140	ALA	2.9
1	K	1	ALA	2.9
1	M	109	ASP	2.9
1	N	26	ASN	2.9
1	J	68	SER	2.8
1	L	125	ASP	2.8
1	J	126	LEU	2.8
1	G	67	LEU	2.8
1	J	122	LYS	2.8
1	J	14	VAL	2.7
1	J	109	ASP	2.7
1	I	96	ASP	2.6
1	M	122	LYS	2.6
1	J	69	ARG	2.6
1	J	28	PRO	2.5
1	G	124	ASP	2.5
1	G	23	LYS	2.5
1	K	122	LYS	2.5
1	K	83	ASP	2.4
1	M	69	ARG	2.4
1	J	25	SER	2.4
1	G	122	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	67	LEU	2.4
1	H	132	GLU	2.4
1	G	83	ASP	2.3
1	M	25	SER	2.3
1	G	25	SER	2.3
1	I	23	LYS	2.3
1	J	78	GLU	2.3
1	M	135	THR	2.3
1	K	124	ASP	2.3
1	K	65	ASN	2.2
1	J	128	LYS	2.2
1	G	66	PRO	2.2
1	N	55	ALA	2.2
1	J	89	ALA	2.2
1	N	72	GLY	2.2
1	H	23	LYS	2.2
1	J	124	ASP	2.2
1	J	131	ASN	2.1
1	H	11	ASP	2.1
1	L	23	LYS	2.1
1	J	91	LYS	2.1
1	G	11	ASP	2.1
1	L	124	ASP	2.1
1	H	153	GLN	2.1
1	G	96	ASP	2.1
1	J	90	ASP	2.1
1	J	94	VAL	2.0
1	I	92	ASP	2.0
1	L	102	SER	2.0
1	N	132	GLU	2.0
1	M	73	GLY	2.0
1	M	76	ASP	2.0
1	J	102	SER	2.0

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

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

6.3 Carbohydrates ⓘ

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.