



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:56 PM EDT

PDB ID : 4KB3 / pdb_00004kb3
Title : Crystal structure of the mitochondrial peroxiredoxin from *Leishmania braziliensis* in the decameric form
Authors : Giuseppe, P.O.; Souza, T.A.C.B.; Morais, M.A.B.; Murakami, M.T.
Deposited on : 2013-04-23
Resolution : 2.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

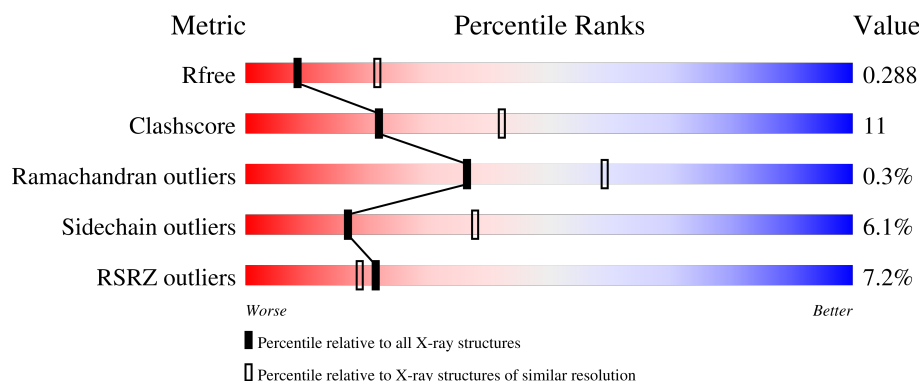
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	192	3% 61% 21% • 15%
1	B	192	8% 63% 23% • 12%
1	C	192	8% 60% 23% • 16%
1	D	192	8% 65% 21% •• 12%
1	E	192	3% 59% 24% • 15%

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Mol	Chain	Length	Quality of chain
1	F	192	3% 57% 26% • 15%
1	G	192	7% 59% 23% • 15%
1	H	192	5% 63% 22% • 12%
1	I	192	9% 58% 25% • 15%
1	J	192	8% 63% 20% •• 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12942 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.

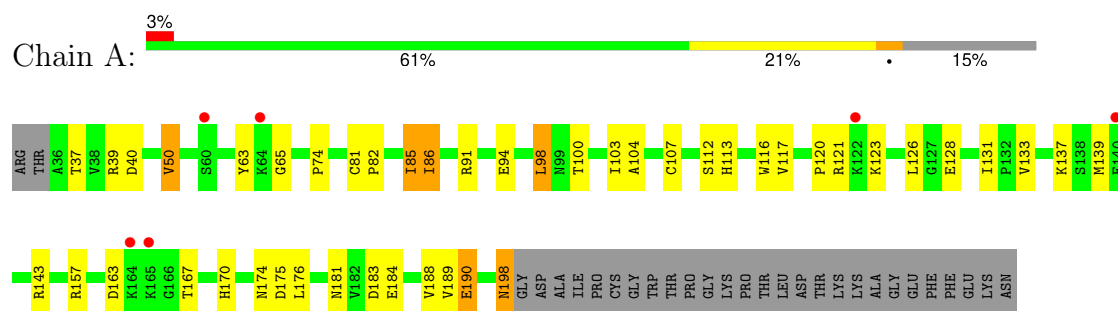
- Molecule 1 is a protein called Peroxidoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	B	169	Total	C	N	O	S	0	0	0
			1321	846	219	250	6			
1	C	162	Total	C	N	O	S	0	0	0
			1275	819	211	240	5			
1	D	169	Total	C	N	O	S	0	0	0
			1321	846	219	250	6			
1	E	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	F	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	G	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	H	169	Total	C	N	O	S	0	0	0
			1327	853	220	248	6			
1	I	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	J	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			

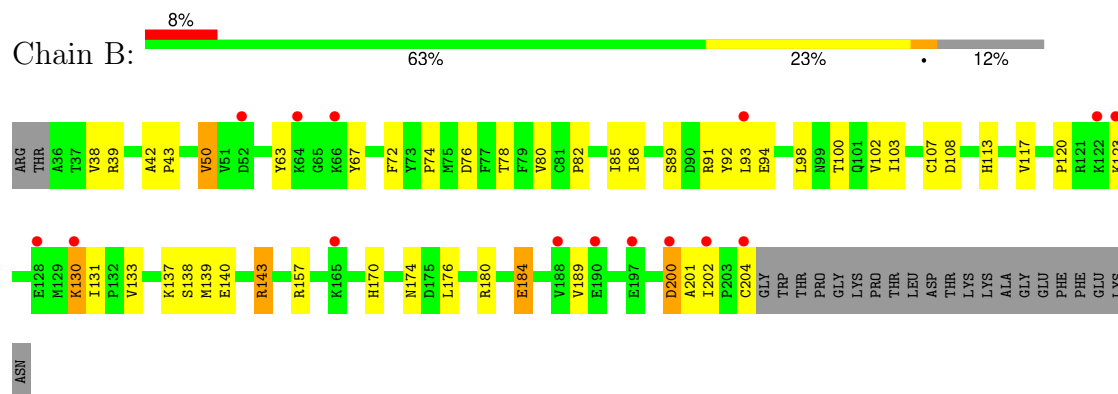
3 Residue-property plots [i](#)

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.

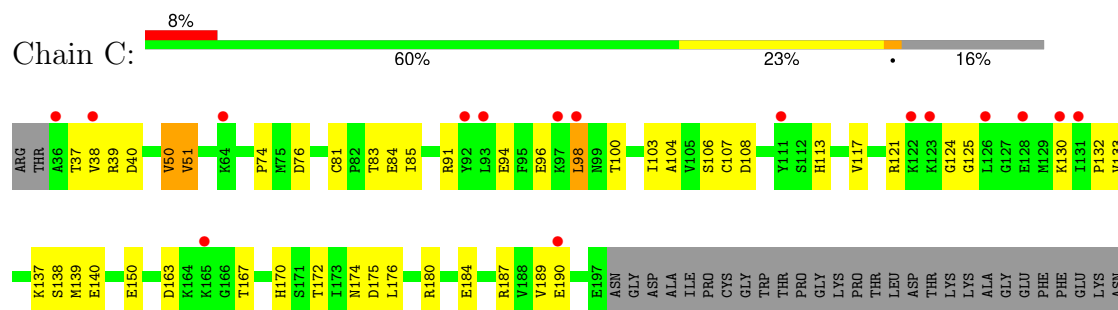
• Molecule 1: Peroxidoxin



• Molecule 1: Peroxidoxin



• Molecule 1: Peroxidoxin

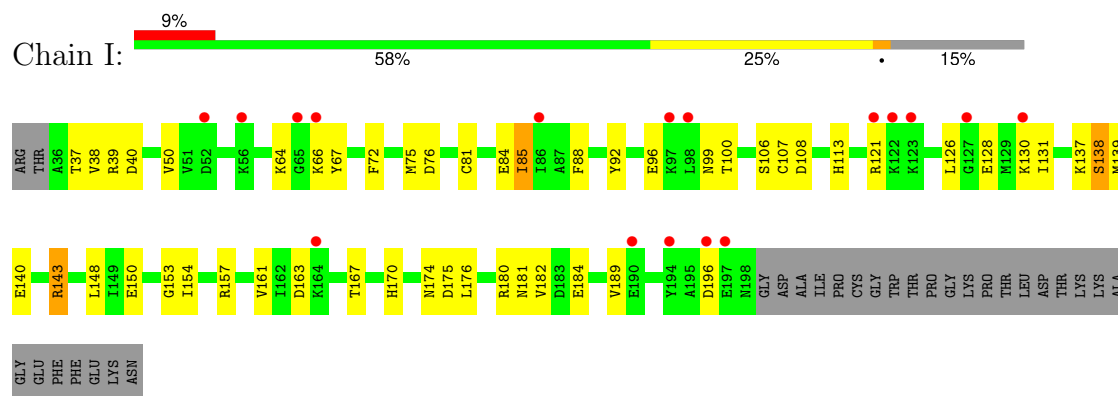


• Molecule 1: Peroxidoxin

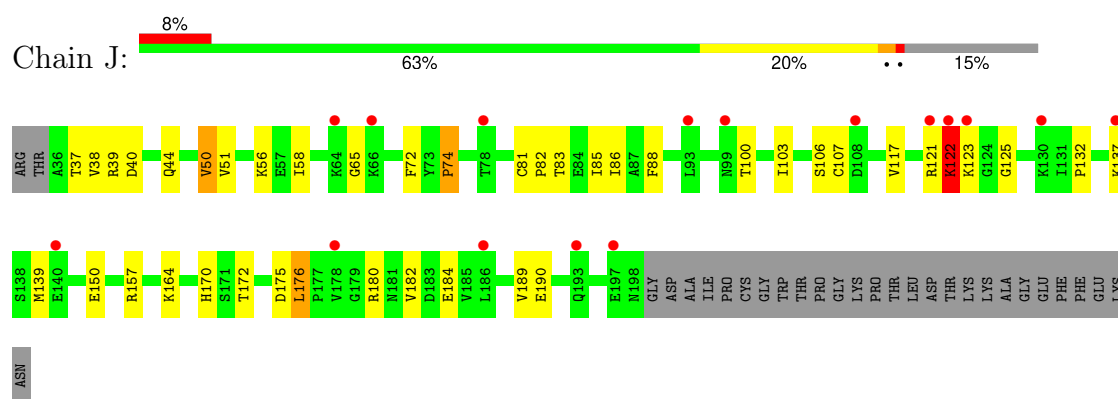




- Molecule 1: Peroxidoxin



- Molecule 1: Peroxidoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.21Å 98.90Å 228.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.93 19.98 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.93) 99.6 (19.98-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.231 , 0.282 0.240 , 0.288	Depositor DCC
R_{free} test set	2432 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12942	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1309	0.89	2/1772 (0.1%)
1	B	0.38	0/1348	0.90	2/1826 (0.1%)
1	C	0.40	0/1301	0.91	2/1761 (0.1%)
1	D	0.42	0/1348	0.94	5/1826 (0.3%)
1	E	0.40	0/1309	0.89	2/1772 (0.1%)
1	F	0.39	0/1309	0.90	1/1772 (0.1%)
1	G	0.41	0/1309	0.87	0/1772
1	H	0.41	0/1355	0.90	3/1835 (0.2%)
1	I	0.38	0/1309	0.91	0/1772
1	J	0.38	0/1309	0.95	3/1772 (0.2%)
All	All	0.40	0/13206	0.91	20/17880 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ILE	CA-C-N	7.33	127.29	120.03
1	D	202	ILE	C-N-CA	7.33	127.29	120.03
1	E	53	GLY	N-CA-C	-6.87	105.75	115.43
1	C	124	GLY	N-CA-C	-5.63	107.24	115.63
1	H	66	LYS	N-CA-C	5.53	118.23	109.50
1	E	65	GLY	N-CA-C	-5.52	107.70	115.32
1	D	178	VAL	N-CA-C	5.45	115.80	108.17
1	J	176	LEU	CA-C-N	-5.38	114.12	119.56
1	J	176	LEU	C-N-CA	-5.38	114.12	119.56
1	F	104	ALA	N-CA-C	-5.38	102.52	110.48
1	J	122	LYS	N-CA-C	-5.31	102.18	110.10
1	D	176	LEU	CA-C-N	-5.30	114.21	119.56
1	D	176	LEU	C-N-CA	-5.30	114.21	119.56
1	A	65	GLY	N-CA-C	-5.29	108.02	115.32
1	B	202	ILE	CA-C-N	5.23	125.17	119.78
1	B	202	ILE	C-N-CA	5.23	125.17	119.78
1	H	65	GLY	N-CA-C	-5.19	106.58	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ALA	N-CA-C	-5.14	102.87	110.48
1	H	166	GLY	N-CA-C	-5.11	108.23	115.43
1	C	104	ALA	N-CA-C	-5.06	102.99	110.48

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	A	1283	0	1279	27	0
1	B	1321	0	1314	34	0
1	C	1275	0	1273	33	0
1	D	1321	0	1314	38	0
1	E	1283	0	1280	33	0
1	F	1283	0	1280	35	0
1	G	1283	0	1279	32	0
1	H	1327	0	1319	29	0
1	I	1283	0	1280	30	0
1	J	1283	0	1280	26	0
All	All	12942	0	12898	276	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 11.

All (276) 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:157:ARG:HB3	1:D:180:ARG:HH22	1.27	0.95
1:F:139:MET:HE2	1:G:139:MET:HE2	1.58	0.83
1:D:139:MET:HE2	1:E:139:MET:HE2	1.65	0.78
1:A:98:LEU:HD21	1:A:190:GLU:HG3	1.67	0.77
1:H:137:LYS:NZ	1:I:107:CYS:O	2.18	0.77
1:I:66:LYS:HZ3	1:I:99:ASN:HA	1.50	0.76
1:B:139:MET:HE2	1:C:139:MET:HE2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:MET:HE2	1:I:139:MET:HE2	1.68	0.74
1:H:100:THR:HG21	1:H:189:VAL:HG11	1.70	0.73
1:E:100:THR:HG21	1:E:189:VAL:HG11	1.72	0.71
1:B:137:LYS:NZ	1:C:107:CYS:O	2.22	0.71
1:H:51:VAL:HG21	1:H:56:LYS:HD3	1.72	0.71
1:B:100:THR:HG21	1:B:189:VAL:HG11	1.72	0.71
1:A:139:MET:HE2	1:J:139:MET:HE2	1.73	0.69
1:E:194:TYR:O	1:E:198:ASN:ND2	2.25	0.69
1:B:107:CYS:O	1:C:137:LYS:NZ	2.23	0.69
1:C:100:THR:HG21	1:C:189:VAL:HG11	1.74	0.69
1:J:100:THR:HG21	1:J:189:VAL:HG11	1.73	0.69
1:D:121:ARG:NH2	1:D:128:GLU:O	2.24	0.68
1:I:100:THR:HG21	1:I:189:VAL:HG11	1.75	0.68
1:G:174:ASN:OD1	1:H:170:HIS:ND1	2.20	0.68
1:D:157:ARG:NH1	1:D:176:LEU:O	2.28	0.67
1:I:121:ARG:NH2	1:I:128:GLU:O	2.26	0.67
1:A:100:THR:HG21	1:A:189:VAL:HG11	1.77	0.67
1:I:138:SER:HB2	1:I:140:GLU:HG2	1.76	0.66
1:G:51:VAL:HG21	1:G:56:LYS:HD3	1.77	0.66
1:C:50:VAL:HG11	1:C:117:VAL:HG21	1.77	0.66
1:D:107:CYS:O	1:E:137:LYS:NZ	2.29	0.65
1:A:137:LYS:NZ	1:J:107:CYS:O	2.30	0.65
1:F:107:CYS:O	1:G:137:LYS:NZ	2.29	0.65
1:B:157:ARG:NH1	1:B:176:LEU:O	2.29	0.64
1:H:107:CYS:O	1:I:137:LYS:NZ	2.30	0.64
1:G:100:THR:HG21	1:G:189:VAL:HG11	1.80	0.63
1:G:170:HIS:ND1	1:H:174:ASN:OD1	2.29	0.63
1:A:50:VAL:HG11	1:A:117:VAL:HG21	1.80	0.62
1:E:174:ASN:OD1	1:F:170:HIS:ND1	2.33	0.62
1:E:157:ARG:NH1	1:E:176:LEU:O	2.33	0.62
1:G:50:VAL:HG11	1:G:117:VAL:HG21	1.83	0.61
1:A:170:HIS:ND1	1:B:174:ASN:OD1	2.28	0.61
1:D:137:LYS:NZ	1:E:107:CYS:O	2.28	0.60
1:J:37:THR:OG1	1:J:38:VAL:N	2.21	0.60
1:C:84:GLU:OE1	1:C:180:ARG:N	2.34	0.60
1:F:100:THR:HG21	1:F:189:VAL:HG11	1.84	0.60
1:D:100:THR:HG21	1:D:189:VAL:HG11	1.82	0.60
1:C:103:ILE:HG12	1:C:132:PRO:HG2	1.83	0.59
1:G:51:VAL:HG12	1:G:132:PRO:HB3	1.84	0.59
1:E:126:LEU:HD13	1:E:129:MET:HE2	1.83	0.59
1:A:74:PRO:HG3	1:A:176:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:THR:HG23	1:D:170:HIS:HE1	1.68	0.59
1:A:120:PRO:HG2	1:A:123:LYS:HG3	1.84	0.58
1:C:76:ASP:OD1	1:C:113:HIS:ND1	2.36	0.58
1:G:80:VAL:HG12	1:H:201:ALA:HB3	1.85	0.58
1:G:113:HIS:CD2	1:G:133:VAL:HG12	2.39	0.58
1:D:157:ARG:CB	1:D:180:ARG:HH22	2.09	0.57
1:D:184:GLU:OE2	1:D:187:ARG:NE	2.28	0.57
1:A:121:ARG:NH2	1:A:128:GLU:O	2.35	0.57
1:F:84:GLU:OE2	1:F:180:ARG:N	2.36	0.57
1:F:108:ASP:HB2	1:F:113:HIS:CE1	2.38	0.57
1:C:51:VAL:HG13	1:C:132:PRO:HB3	1.86	0.57
1:E:63:TYR:CE2	1:E:103:ILE:HD11	2.39	0.57
1:H:157:ARG:NH1	1:H:176:LEU:O	2.36	0.56
1:A:107:CYS:O	1:J:137:LYS:NZ	2.38	0.56
1:G:97:LYS:HG2	1:G:98:LEU:HD12	1.88	0.56
1:I:157:ARG:NH1	1:I:176:LEU:O	2.36	0.56
1:I:38:VAL:O	1:I:39:ARG:HB2	2.06	0.55
1:A:198:ASN:OD1	1:A:198:ASN:N	2.40	0.55
1:H:143:ARG:HG3	1:H:148:LEU:HD23	1.87	0.55
1:B:108:ASP:HB2	1:B:113:HIS:CE1	2.42	0.55
1:D:71:PHE:CE1	1:D:85:ILE:HG13	2.42	0.55
1:F:138:SER:OG	1:F:140:GLU:HB2	2.07	0.55
1:J:157:ARG:NH1	1:J:176:LEU:O	2.39	0.54
1:A:175:ASP:OD1	1:A:176:LEU:N	2.40	0.54
1:B:200:ASP:OD1	1:B:201:ALA:N	2.41	0.54
1:C:38:VAL:O	1:C:39:ARG:HB2	2.07	0.54
1:A:85:ILE:HD12	1:A:85:ILE:H	1.72	0.54
1:C:94:GLU:O	1:C:98:LEU:HD12	2.07	0.54
1:C:184:GLU:OE2	1:C:187:ARG:NH2	2.36	0.54
1:B:38:VAL:O	1:B:39:ARG:HB2	2.07	0.54
1:D:200:ASP:OD2	1:D:200:ASP:N	2.40	0.54
1:E:193:GLN:O	1:E:197:GLU:HG3	2.08	0.54
1:I:67:TYR:OH	1:I:196:ASP:OD2	2.26	0.54
1:F:51:VAL:HG13	1:F:56:LYS:HB3	1.88	0.54
1:B:108:ASP:HB2	1:B:113:HIS:HE1	1.73	0.53
1:B:184:GLU:OE2	1:B:184:GLU:HA	2.08	0.53
1:G:184:GLU:HG2	1:H:184:GLU:HG2	1.90	0.53
1:A:121:ARG:NE	1:A:126:LEU:O	2.37	0.53
1:C:163:ASP:OD2	1:C:167:THR:N	2.39	0.53
1:I:88:PHE:CE2	1:I:182:VAL:HG22	2.43	0.53
1:E:50:VAL:HG11	1:E:117:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG22	1:D:132:PRO:HB3	1.91	0.53
1:J:65:GLY:O	1:J:164:LYS:HE3	2.09	0.53
1:J:175:ASP:OD2	1:J:176:LEU:N	2.41	0.52
1:I:75:MET:HE2	1:I:154:ILE:HG21	1.92	0.52
1:J:50:VAL:HG11	1:J:117:VAL:HG21	1.91	0.52
1:D:74:PRO:HG3	1:D:176:LEU:HD22	1.91	0.52
1:C:108:ASP:HB2	1:C:113:HIS:CE1	2.44	0.52
1:G:184:GLU:OE1	1:G:184:GLU:HA	2.10	0.52
1:I:121:ARG:NE	1:I:126:LEU:O	2.41	0.52
1:F:108:ASP:HB2	1:F:113:HIS:HE1	1.74	0.52
1:I:143:ARG:HG3	1:I:148:LEU:HD23	1.91	0.52
1:J:38:VAL:O	1:J:39:ARG:HB2	2.10	0.52
1:E:72:PHE:O	1:E:180:ARG:NH2	2.36	0.52
1:G:38:VAL:O	1:G:39:ARG:HB2	2.07	0.52
1:E:163:ASP:OD1	1:E:167:THR:N	2.43	0.52
1:H:38:VAL:O	1:H:39:ARG:HB2	2.09	0.52
1:F:74:PRO:HG3	1:F:176:LEU:HD22	1.91	0.51
1:F:143:ARG:HG3	1:F:148:LEU:HD23	1.92	0.51
1:C:113:HIS:CD2	1:C:133:VAL:HG12	2.45	0.51
1:E:170:HIS:NE2	1:E:172:THR:OG1	2.39	0.51
1:A:82:PRO:O	1:A:86:ILE:HG13	2.10	0.51
1:D:121:ARG:NE	1:D:126:LEU:O	2.35	0.51
1:F:181:ASN:OD1	1:F:184:GLU:N	2.33	0.51
1:F:193:GLN:O	1:F:197:GLU:HG3	2.11	0.51
1:I:163:ASP:OD2	1:I:167:THR:N	2.42	0.51
1:H:82:PRO:O	1:H:86:ILE:HG13	2.11	0.51
1:B:92:TYR:CZ	1:B:93:LEU:HG	2.46	0.51
1:I:175:ASP:OD1	1:I:176:LEU:N	2.44	0.51
1:A:157:ARG:NH1	1:A:176:LEU:O	2.41	0.50
1:A:184:GLU:HG2	1:B:184:GLU:HG2	1.93	0.50
1:D:92:TYR:CZ	1:D:93:LEU:HG	2.47	0.50
1:F:38:VAL:O	1:F:39:ARG:HB2	2.11	0.50
1:I:76:ASP:OD1	1:I:113:HIS:ND1	2.35	0.50
1:C:174:ASN:OD1	1:D:170:HIS:ND1	2.41	0.50
1:E:63:TYR:HE2	1:E:103:ILE:HD11	1.76	0.50
1:B:120:PRO:HG2	1:B:123:LYS:HG3	1.92	0.50
1:D:94:GLU:O	1:D:98:LEU:HD13	2.11	0.50
1:H:74:PRO:HG3	1:H:176:LEU:HD22	1.93	0.50
1:B:50:VAL:HG11	1:B:117:VAL:HG21	1.92	0.50
1:A:163:ASP:OD2	1:A:167:THR:N	2.41	0.50
1:C:170:HIS:ND1	1:D:174:ASN:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:TYR:OH	1:F:196:ASP:OD2	2.27	0.49
1:D:198:ASN:OD1	1:D:198:ASN:N	2.43	0.49
1:E:38:VAL:O	1:E:39:ARG:HB2	2.12	0.49
1:F:137:LYS:NZ	1:G:107:CYS:O	2.44	0.49
1:J:72:PHE:O	1:J:180:ARG:NH2	2.42	0.49
1:D:157:ARG:HB3	1:D:180:ARG:NH2	2.11	0.49
1:I:37:THR:OG1	1:I:40:ASP:OD2	2.29	0.49
1:E:143:ARG:HG3	1:E:148:LEU:HD23	1.94	0.49
1:C:81:CYS:SG	1:D:204:CYS:N	2.82	0.49
1:E:175:ASP:HB3	1:F:192:PHE:HE1	1.78	0.48
1:C:175:ASP:HB3	1:D:192:PHE:HE1	1.78	0.48
1:C:91:ARG:NH2	1:C:94:GLU:OE1	2.46	0.48
1:B:91:ARG:NE	1:B:94:GLU:OE1	2.37	0.48
1:E:121:ARG:NE	1:E:126:LEU:O	2.42	0.48
1:G:184:GLU:OE2	1:G:187:ARG:NH2	2.39	0.48
1:D:102:VAL:HB	1:D:131:ILE:HG21	1.96	0.48
1:I:184:GLU:CD	1:J:184:GLU:HG3	2.38	0.48
1:J:122:LYS:O	1:J:123:LYS:HB2	2.13	0.48
1:C:138:SER:OG	1:C:140:GLU:HB2	2.14	0.48
1:B:85:ILE:HD12	1:B:85:ILE:H	1.77	0.47
1:B:137:LYS:HZ1	1:C:107:CYS:C	2.20	0.47
1:F:184:GLU:O	1:F:188:VAL:HG13	2.13	0.47
1:A:184:GLU:O	1:A:188:VAL:HG23	2.14	0.47
1:G:163:ASP:OD1	1:G:167:THR:N	2.43	0.47
1:F:113:HIS:CD2	1:F:133:VAL:HG12	2.50	0.47
1:I:163:ASP:OD1	1:I:167:THR:OG1	2.31	0.47
1:B:113:HIS:CD2	1:B:133:VAL:HG12	2.49	0.47
1:F:161:VAL:HB	1:F:170:HIS:HB3	1.97	0.47
1:A:91:ARG:NH2	1:A:183:ASP:OD1	2.40	0.47
1:A:174:ASN:OD1	1:B:170:HIS:ND1	2.42	0.47
1:B:89:SER:HG	1:B:130:LYS:H	1.62	0.47
1:C:37:THR:OG1	1:C:40:ASP:OD1	2.31	0.47
1:C:184:GLU:CD	1:D:184:GLU:HG3	2.39	0.47
1:F:64:LYS:HA	1:F:64:LYS:HD3	1.56	0.47
1:F:163:ASP:OD1	1:F:167:THR:N	2.45	0.47
1:J:122:LYS:H	1:J:122:LYS:HG2	1.22	0.47
1:D:63:TYR:HE2	1:D:103:ILE:HD11	1.78	0.47
1:B:76:ASP:OD1	1:B:113:HIS:ND1	2.47	0.47
1:C:85:ILE:H	1:C:85:ILE:HD12	1.79	0.47
1:E:37:THR:HG22	1:E:40:ASP:OD2	2.15	0.47
1:D:85:ILE:HD12	1:D:85:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:HIS:NE2	1:J:172:THR:OG1	2.42	0.47
1:E:175:ASP:OD1	1:E:176:LEU:N	2.47	0.46
1:C:108:ASP:HB2	1:C:113:HIS:HE1	1.81	0.46
1:E:84:GLU:OE2	1:E:180:ARG:N	2.45	0.46
1:E:184:GLU:OE2	1:E:187:ARG:NH2	2.42	0.46
1:G:67:TYR:HB2	1:G:100:THR:HG22	1.97	0.46
1:H:63:TYR:CE2	1:H:103:ILE:HD11	2.51	0.46
1:G:51:VAL:HG23	1:G:52:ASP:H	1.81	0.46
1:H:184:GLU:O	1:H:188:VAL:HG23	2.15	0.46
1:I:181:ASN:HB3	1:J:184:GLU:OE2	2.16	0.46
1:C:184:GLU:CG	1:D:184:GLU:HG3	2.45	0.46
1:H:175:ASP:OD1	1:H:176:LEU:N	2.48	0.46
1:D:121:ARG:HA	1:D:125:GLY:O	2.15	0.46
1:A:181:ASN:OD1	1:A:184:GLU:N	2.40	0.45
1:F:103:ILE:HG12	1:F:132:PRO:HG2	1.98	0.45
1:F:185:VAL:O	1:F:188:VAL:HG22	2.16	0.45
1:G:74:PRO:C	1:G:75:MET:HG3	2.40	0.45
1:B:140:GLU:OE1	1:B:143:ARG:NH1	2.49	0.45
1:F:82:PRO:O	1:F:86:ILE:HG13	2.17	0.45
1:F:126:LEU:HD22	1:F:129:MET:HE2	1.97	0.45
1:G:181:ASN:OD1	1:G:184:GLU:N	2.38	0.45
1:G:185:VAL:O	1:G:188:VAL:HG22	2.15	0.45
1:I:92:TYR:CE2	1:I:130:LYS:HD2	2.52	0.45
1:B:78:THR:HB	1:B:80:VAL:HG22	1.99	0.45
1:I:84:GLU:HG3	1:I:85:ILE:N	2.32	0.45
1:I:106:SER:OG	1:I:107:CYS:N	2.50	0.45
1:A:94:GLU:O	1:A:98:LEU:HD12	2.17	0.45
1:H:76:ASP:OD1	1:H:113:HIS:ND1	2.41	0.45
1:E:175:ASP:HB3	1:F:192:PHE:CE1	2.52	0.44
1:G:138:SER:OG	1:G:140:GLU:HB2	2.17	0.44
1:A:37:THR:OG1	1:A:40:ASP:OD2	2.34	0.44
1:B:63:TYR:HE2	1:B:103:ILE:HD11	1.82	0.44
1:B:138:SER:OG	1:B:140:GLU:HG2	2.16	0.44
1:H:108:ASP:HB2	1:H:113:HIS:CE1	2.51	0.44
1:J:37:THR:O	1:J:40:ASP:HB2	2.17	0.44
1:C:172:THR:HG23	1:D:170:HIS:CE1	2.51	0.44
1:D:67:TYR:HB2	1:D:100:THR:HG22	1.99	0.44
1:C:121:ARG:HA	1:C:125:GLY:O	2.18	0.44
1:H:63:TYR:HE2	1:H:103:ILE:HD11	1.82	0.44
1:J:88:PHE:CE2	1:J:182:VAL:HG22	2.53	0.44
1:J:121:ARG:HA	1:J:125:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TYR:CE2	1:B:103:ILE:HD11	2.53	0.44
1:I:161:VAL:HB	1:I:170:HIS:HB3	1.99	0.44
1:J:37:THR:HG1	1:J:38:VAL:H	1.57	0.44
1:G:74:PRO:HG3	1:G:176:LEU:HD22	2.00	0.43
1:E:64:LYS:HD2	1:E:64:LYS:HA	1.83	0.43
1:E:88:PHE:CE2	1:E:182:VAL:HG22	2.52	0.43
1:F:137:LYS:HE3	1:G:153:GLY:O	2.19	0.43
1:D:175:ASP:OD2	1:D:176:LEU:N	2.48	0.43
1:E:185:VAL:O	1:E:188:VAL:HG22	2.18	0.43
1:B:67:TYR:HB2	1:B:100:THR:HG22	2.00	0.43
1:G:175:ASP:OD1	1:G:176:LEU:N	2.48	0.43
1:G:61:ASN:O	1:G:64:LYS:HG3	2.19	0.43
1:G:163:ASP:OD2	1:G:167:THR:OG1	2.37	0.43
1:H:85:ILE:HG22	1:H:129:MET:HE1	1.99	0.43
1:C:74:PRO:HG3	1:C:176:LEU:HD22	2.00	0.43
1:D:38:VAL:O	1:D:39:ARG:HB2	2.18	0.43
1:D:157:ARG:HD2	1:D:176:LEU:O	2.19	0.43
1:H:137:LYS:HE3	1:I:153:GLY:O	2.19	0.43
1:H:197:GLU:HG3	1:H:198:ASN:OD1	2.19	0.43
1:B:74:PRO:HG3	1:B:176:LEU:HD22	2.00	0.43
1:B:82:PRO:O	1:B:86:ILE:HG12	2.19	0.43
1:B:72:PHE:O	1:B:180:ARG:NH2	2.51	0.42
1:J:51:VAL:HG21	1:J:56:LYS:HD3	2.01	0.42
1:J:103:ILE:HG12	1:J:132:PRO:HG2	2.01	0.42
1:J:74:PRO:HG3	1:J:176:LEU:HD22	2.01	0.42
1:D:137:LYS:HD2	1:D:137:LYS:HA	1.80	0.42
1:C:106:SER:OG	1:C:107:CYS:N	2.53	0.42
1:I:108:ASP:HB2	1:I:113:HIS:CE1	2.55	0.42
1:A:63:TYR:CE2	1:A:103:ILE:HD11	2.54	0.42
1:E:103:ILE:HG12	1:E:132:PRO:HG2	2.00	0.42
1:G:44:GLN:HG2	1:G:60:SER:HB3	2.01	0.42
1:H:51:VAL:HG12	1:H:132:PRO:HB3	2.01	0.42
1:B:102:VAL:HB	1:B:131:ILE:HD13	2.00	0.42
1:E:37:THR:O	1:E:40:ASP:HB2	2.20	0.42
1:F:41:PRO:HA	1:F:167:THR:HA	2.01	0.42
1:I:174:ASN:OD1	1:J:170:HIS:ND1	2.53	0.42
1:D:64:LYS:HA	1:D:64:LYS:HD2	1.75	0.42
1:F:55:ILE:HG13	1:F:114:LEU:HD22	2.02	0.41
1:A:113:HIS:CD2	1:A:133:VAL:HG12	2.56	0.41
1:B:42:ALA:HA	1:B:43:PRO:HD3	1.93	0.41
1:E:189:VAL:O	1:E:193:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:VAL:HG23	1:G:52:ASP:N	2.36	0.41
1:H:71:PHE:HD1	1:H:159:LEU:HD12	1.84	0.41
1:C:175:ASP:HB3	1:D:192:PHE:CE1	2.54	0.41
1:F:120:PRO:HG2	1:F:123:LYS:HG3	2.02	0.41
1:A:63:TYR:HE2	1:A:103:ILE:HD11	1.86	0.41
1:G:143:ARG:HG3	1:G:148:LEU:HD23	2.02	0.41
1:F:160:PHE:CE1	1:F:171:SER:HB2	2.56	0.41
1:I:72:PHE:O	1:I:180:ARG:NH2	2.47	0.41
1:F:189:VAL:O	1:F:193:GLN:HG3	2.20	0.41
1:E:161:VAL:HB	1:E:170:HIS:HB3	2.03	0.41
1:F:137:LYS:HA	1:F:137:LYS:HD2	1.84	0.41
1:H:137:LYS:HZ1	1:I:107:CYS:C	2.24	0.41
1:H:161:VAL:HB	1:H:170:HIS:HB3	2.02	0.41
1:B:170:HIS:CD2	1:B:170:HIS:C	2.99	0.41
1:D:161:VAL:HB	1:D:170:HIS:HB3	2.03	0.41
1:H:50:VAL:HG11	1:H:117:VAL:HG21	2.03	0.41
1:H:84:GLU:OE2	1:H:180:ARG:N	2.53	0.41
1:J:82:PRO:O	1:J:86:ILE:HG12	2.21	0.40
1:E:106:SER:OG	1:E:107:CYS:N	2.53	0.40
1:F:170:HIS:CD2	1:F:170:HIS:C	2.99	0.40
1:J:106:SER:OG	1:J:107:CYS:N	2.54	0.40
1:G:84:GLU:OE2	1:G:180:ARG:N	2.52	0.40
1:E:51:VAL:HG23	1:E:52:ASP:H	1.87	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	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	B	167/192 (87%)	158 (95%)	8 (5%)	1 (1%)	21	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	160/192 (83%)	156 (98%)	4 (2%)	0	100	100
1	D	167/192 (87%)	159 (95%)	5 (3%)	3 (2%)	6	19
1	E	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	F	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	G	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	H	165/192 (86%)	161 (98%)	4 (2%)	0	100	100
1	I	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	J	161/192 (84%)	155 (96%)	5 (3%)	1 (1%)	21	45
All	All	1625/1920 (85%)	1574 (97%)	46 (3%)	5 (0%)	36	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	ASP
1	D	199	GLY
1	B	200	ASP
1	J	74	PRO
1	D	74	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	A	139/162 (86%)	127 (91%)	12 (9%)	10	24
1	B	143/162 (88%)	137 (96%)	6 (4%)	26	52
1	C	138/162 (85%)	130 (94%)	8 (6%)	18	40
1	D	143/162 (88%)	138 (96%)	5 (4%)	32	56
1	E	139/162 (86%)	133 (96%)	6 (4%)	26	51
1	F	139/162 (86%)	130 (94%)	9 (6%)	15	35
1	G	139/162 (86%)	129 (93%)	10 (7%)	13	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	143/162 (88%)	132 (92%)	11 (8%)	12	28
1	I	139/162 (86%)	130 (94%)	9 (6%)	15	35
1	J	139/162 (86%)	130 (94%)	9 (6%)	15	35
All	All	1401/1620 (86%)	1316 (94%)	85 (6%)	17	38

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	50	VAL
1	A	81	CYS
1	A	85	ILE
1	A	86	ILE
1	A	98	LEU
1	A	112	SER
1	A	116	TRP
1	A	131	ILE
1	A	143	ARG
1	A	190	GLU
1	A	198	ASN
1	B	50	VAL
1	B	98	LEU
1	B	130	LYS
1	B	143	ARG
1	B	184	GLU
1	B	204	CYS
1	C	50	VAL
1	C	51	VAL
1	C	83	THR
1	C	96	GLU
1	C	98	LEU
1	C	130	LYS
1	C	150	GLU
1	C	190	GLU
1	D	96	GLU
1	D	140	GLU
1	D	196	ASP
1	D	198	ASN
1	D	200	ASP
1	E	50	VAL
1	E	85	ILE

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Mol	Chain	Res	Type
1	E	143	ARG
1	E	150	GLU
1	E	190	GLU
1	E	198	ASN
1	F	37	THR
1	F	50	VAL
1	F	51	VAL
1	F	80	VAL
1	F	85	ILE
1	F	86	ILE
1	F	100	THR
1	F	140	GLU
1	F	190	GLU
1	G	44	GLN
1	G	50	VAL
1	G	66	LYS
1	G	81	CYS
1	G	85	ILE
1	G	143	ARG
1	G	150	GLU
1	G	184	GLU
1	G	190	GLU
1	G	198	ASN
1	H	48	LYS
1	H	81	CYS
1	H	85	ILE
1	H	86	ILE
1	H	98	LEU
1	H	100	THR
1	H	143	ARG
1	H	150	GLU
1	H	197	GLU
1	H	202	ILE
1	H	204	CYS
1	I	50	VAL
1	I	64	LYS
1	I	81	CYS
1	I	85	ILE
1	I	96	GLU
1	I	131	ILE
1	I	138	SER
1	I	143	ARG

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Mol	Chain	Res	Type
1	I	150	GLU
1	J	44	GLN
1	J	50	VAL
1	J	58	ILE
1	J	81	CYS
1	J	83	THR
1	J	85	ILE
1	J	122	LYS
1	J	150	GLU
1	J	190	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	ASN
1	F	193	GLN
1	H	44	GLN
1	H	61	ASN
1	J	193	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	A	163/192 (84%)	0.33	6 (3%) 45 36	42, 78, 105, 136	10 (6%)
1	B	169/192 (88%)	0.45	15 (8%) 15 14	39, 79, 102, 176	18 (10%)
1	C	162/192 (84%)	0.61	16 (9%) 13 12	39, 80, 111, 149	21 (12%)
1	D	169/192 (88%)	0.54	16 (9%) 14 13	34, 83, 110, 146	18 (10%)
1	E	163/192 (84%)	0.30	6 (3%) 45 36	40, 78, 101, 122	11 (6%)
1	F	163/192 (84%)	0.39	5 (3%) 51 43	43, 77, 101, 122	14 (8%)
1	G	163/192 (84%)	0.67	13 (7%) 18 16	38, 76, 99, 121	14 (8%)
1	H	169/192 (88%)	0.68	9 (5%) 32 26	33, 77, 107, 158	13 (7%)
1	I	163/192 (84%)	0.47	17 (10%) 11 11	42, 77, 102, 134	24 (14%)
1	J	163/192 (84%)	0.52	16 (9%) 13 12	44, 78, 120, 152	21 (12%)
All	All	1647/1920 (85%)	0.50	119 (7%) 21 19	33, 78, 107, 176	164 (9%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	GLU	7.4
1	B	64	LYS	6.1
1	C	190	GLU	6.1
1	J	93	LEU	5.9
1	I	190	GLU	5.9
1	E	97	LYS	5.8
1	C	165	LYS	5.8
1	B	128	GLU	5.7
1	A	64	LYS	5.6
1	J	197	GLU	5.4
1	C	64	LYS	5.3
1	G	128	GLU	5.2
1	H	140	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	200	ASP	5.1
1	A	164	LYS	5.1
1	B	130	LYS	5.0
1	D	140	GLU	4.9
1	I	97	LYS	4.9
1	B	66	LYS	4.7
1	C	128	GLU	4.7
1	I	52	ASP	4.4
1	I	197	GLU	4.4
1	B	165	LYS	4.3
1	D	202	ILE	4.3
1	H	123	LYS	4.2
1	J	99	ASN	4.2
1	D	123	LYS	4.1
1	A	122	LYS	4.0
1	B	122	LYS	4.0
1	J	186	LEU	4.0
1	B	190	GLU	4.0
1	G	197	GLU	4.0
1	C	123	LYS	3.9
1	D	164	LYS	3.9
1	D	190	GLU	3.9
1	B	197	GLU	3.8
1	J	66	LYS	3.8
1	C	92	TYR	3.7
1	J	140	GLU	3.7
1	C	130	LYS	3.7
1	C	126	LEU	3.7
1	G	97	LYS	3.7
1	H	201	ALA	3.6
1	E	122	LYS	3.6
1	E	140	GLU	3.5
1	D	197	GLU	3.5
1	G	123	LYS	3.4
1	B	202	ILE	3.4
1	F	165	LYS	3.4
1	J	123	LYS	3.4
1	B	123	LYS	3.3
1	H	206	TRP	3.3
1	D	97	LYS	3.3
1	C	131	ILE	3.3
1	E	80	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	56	LYS	3.2
1	B	204	CYS	3.2
1	I	123	LYS	3.2
1	A	60	SER	3.1
1	I	121	ARG	3.1
1	D	48	LYS	3.1
1	A	165	LYS	3.1
1	C	97	LYS	3.1
1	J	121	ARG	3.0
1	C	111	TYR	3.0
1	D	122	LYS	3.0
1	I	86	ILE	3.0
1	I	122	LYS	3.0
1	J	122	LYS	2.9
1	G	124	GLY	2.9
1	I	196	ASP	2.9
1	J	193	GLN	2.9
1	A	140	GLU	2.9
1	F	190	GLU	2.9
1	I	130	LYS	2.9
1	H	97	LYS	2.8
1	D	165	LYS	2.8
1	G	122	LYS	2.8
1	J	178	VAL	2.8
1	I	98	LEU	2.8
1	H	80	VAL	2.7
1	B	52	ASP	2.7
1	C	93	LEU	2.7
1	G	165	LYS	2.6
1	H	93	LEU	2.6
1	D	130	LYS	2.5
1	I	66	LYS	2.5
1	E	66	LYS	2.5
1	I	56	LYS	2.5
1	H	205	GLY	2.4
1	C	122	LYS	2.4
1	G	71	PHE	2.4
1	C	36	ALA	2.4
1	C	38	VAL	2.4
1	J	108	ASP	2.4
1	E	93	LEU	2.3
1	G	67	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	VAL	2.3
1	C	98	LEU	2.3
1	J	137	LYS	2.2
1	I	194	TYR	2.2
1	B	93	LEU	2.2
1	G	80	VAL	2.2
1	I	127	GLY	2.2
1	F	97	LYS	2.2
1	I	65	GLY	2.2
1	J	78	THR	2.2
1	J	130	LYS	2.2
1	D	60	SER	2.2
1	B	200	ASP	2.1
1	H	196	ASP	2.1
1	F	81	CYS	2.1
1	G	140	GLU	2.1
1	D	176	LEU	2.1
1	G	96	GLU	2.1
1	F	122	LYS	2.0
1	G	85	ILE	2.0
1	I	164	LYS	2.0
1	J	64	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.