Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 04:16 am GMT

PDB ID	:	2BJY
Title	:	The X-ray crystal structure of Listeria innocua Dps H31G-H43G mutant.
Authors	:	Ilari, A.; Stefanini, S.; Chiancone, E.
Deposited on	:	2005-02-08
Resolution	:	2.60 Å(reported)

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

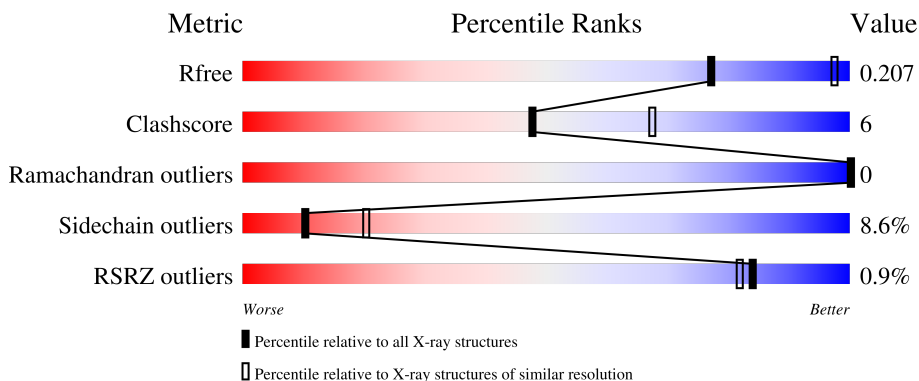|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	Percentile Ranks	Value
Rfree		0.207
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		8.6%
RSRZ outliers		0.9%

Worse ⟷ *Better*

▋ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	156	3% · 79% · 13% · ·
1	B	156	% · 74% · 19% · · ·
1	C	156	80% · 12% · · ·
1	D	156	2% · 81% · 12% · · ·
1	E	156	% · 81% · 10% · · ·

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	156	77% 14%
1	G	156	81% 12%
1	H	156	72% 18% 5%
1	I	156	76% 16%
1	J	156	72% 19%
1	K	156	74% 18%
1	L	156	79% 13%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 14696 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 NON-HEME IRON-CONTAINING FERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	B	151	Total	C	N	O	S	0	0	0
			1216	779	193	237	7			
1	C	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	D	150	Total	C	N	O	S	0	1	0
			1214	778	192	237	7			
1	E	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	F	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	G	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	H	149	Total	C	N	O	S	0	1	0
			1207	773	191	236	7			
1	I	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	J	150	Total	C	N	O	S	0	0	0
			1210	776	192	235	7			
1	K	149	Total	C	N	O	S	0	0	0
			1203	771	191	234	7			
1	L	152	Total	C	N	O	S	0	0	0
			1224	783	195	239	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	HIS	engineered mutation	UNP P80725
A	43	GLY	HIS	engineered mutation	UNP P80725
B	31	GLY	HIS	engineered mutation	UNP P80725
B	43	GLY	HIS	engineered mutation	UNP P80725
C	31	GLY	HIS	engineered mutation	UNP P80725

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Chain	Residue	Modelled	Actual	Comment	Reference
C	43	GLY	HIS	engineered mutation	UNP P80725
D	31	GLY	HIS	engineered mutation	UNP P80725
D	43	GLY	HIS	engineered mutation	UNP P80725
E	31	GLY	HIS	engineered mutation	UNP P80725
E	43	GLY	HIS	engineered mutation	UNP P80725
F	31	GLY	HIS	engineered mutation	UNP P80725
F	43	GLY	HIS	engineered mutation	UNP P80725
G	31	GLY	HIS	engineered mutation	UNP P80725
G	43	GLY	HIS	engineered mutation	UNP P80725
H	31	GLY	HIS	engineered mutation	UNP P80725
H	43	GLY	HIS	engineered mutation	UNP P80725
I	31	GLY	HIS	engineered mutation	UNP P80725
I	43	GLY	HIS	engineered mutation	UNP P80725
J	31	GLY	HIS	engineered mutation	UNP P80725
J	43	GLY	HIS	engineered mutation	UNP P80725
K	31	GLY	HIS	engineered mutation	UNP P80725
K	43	GLY	HIS	engineered mutation	UNP P80725
L	31	GLY	HIS	engineered mutation	UNP P80725
L	43	GLY	HIS	engineered mutation	UNP P80725

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	14	Total 14	O 14	0	0
2	C	13	Total 13	O 13	0	0
2	D	17	Total 17	O 17	0	0
2	E	16	Total 16	O 16	0	0
2	F	8	Total 8	O 8	0	0
2	G	11	Total 11	O 11	0	0
2	H	25	Total 25	O 25	0	0
2	I	11	Total 11	O 11	0	0
2	J	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	9	Total　O 9　　9	0	0
2	L	14	Total　O 14　　14	0	0

3 Residue-property plots ⓘ

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: NON-HEME IRON-CONTAINING FERRITIN

Chain A:

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain B:

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain C:

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain D:

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain E:

MET LYS THR ILE ASN SER V7 L13 L20 T24 Q29 W32 Y33 M34 N38 L42 K45 E55 Q56 M57 L65 S73 T94 M95 L102 D111 G116 T120 D121 N129 L132 P154 L155 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain F:

%

77%   14%   • • •

MET LYS THR ILE ASN SER V7 L13 L20 T24 I30 G31 W32 Y33 M34 H37 N38 T41 L42 M57 E62 L65 A66 P71 F72 S73 T74 L75 K76 E77 M95 M99 L102 K114 Q115 G116 T120 N129 L132 L150 G151 K152

E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain G:

81%   12%   • • •

MET LYS THR ILE ASN SER V7 L13 L20 T24 Q29 L42 Y50 E55 L65 S73 T94 M95 D96 L102 G116 L119 T120 D121 T128 N129 D130 M131 L132 K147 K152 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain H:

72%   18%   5% • •

MET LYS THR ILE ASN SER VAL D8 T9 L13 N14 L20 T24 I27 I30 G31 W32 Y33 M34 R35 G36 H37 L49 Y50 E55 Q56 M57 D58 L65 P71 E80 V84 P88 T94 M95 D96 Q97 L98 M99 L102 T105 T120 E123

N129 D130 M131 L132 K136 F149 P154 L155 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain I:

2%

76%   16%   • • •

MET LYS THR ILE ASN SER V7 E11 F12 L13 N14 H15 L20 T24 Q29 I30 G31 W32 Y33 M34 H37 L42 K45 L49 E52 D58 L64 L65 G69 S73 S83 K91 D96 M99 L102 E118 L119 D130 M131 L132

S138 A153 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain J:

72%   19%   • • •

MET LYS THR ILE ASN SER V7 D8 L13 N14 H15 L20 T24 V25 K26 Q29 I30 H37 N38 T41 L42 K45 S51 E55 Q56 M57 L65 P71 L75 S83 D96 M99 E100 D101 L102 T105 K114 Q115 G116 I117 E118 L119 T120

D121 K122 T128 N129 L132 K152 A153 P154 L155 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain K:

MET LYS THR ILE ASN SER VAL D8 F12 L20 T24 Q29 H37 N38 F39 F40 K45 Y50 D58 L65 A66 P71 F72 S73 T74 E77 T90 T94 M95 D96 E100 D101 L102 V103 G116 L119 T120 D121 K122 E123 G124 D125 N129

L132 D140 K141 G151 P154 L155 E156

• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain L:

MET LYS THR ILE N5 L13 L20 N21 V22 F23 T24 L42 K45 Y50 M57 D58 L65 P71 F72 S73 K91 P92 K93 T94 M95 D96 D101 L102 R110 G116 T120 N129 L132 K147 K152 A153 P154 L155 E156

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.62Å　　132.21Å　　168.04Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	30.00　–　2.60 19.99　–　2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.60) 93.9 (19.99-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.207　,　0.252 0.208　,　0.207	Depositor DCC
R_{free} test set	2863 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 26.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14696	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.93	0/1235	1.08	3/1664 (0.2%)
1	B	0.98	2/1241 (0.2%)	1.11	5/1672 (0.3%)
1	C	0.94	1/1235 (0.1%)	1.04	3/1664 (0.2%)
1	D	0.97	0/1243	1.03	3/1675 (0.2%)
1	E	0.95	1/1235 (0.1%)	1.06	6/1664 (0.4%)
1	F	0.96	4/1235 (0.3%)	1.08	3/1664 (0.2%)
1	G	0.91	0/1235	1.05	5/1664 (0.3%)
1	H	0.93	1/1236 (0.1%)	1.14	7/1665 (0.4%)
1	I	0.93	0/1235	1.14	8/1664 (0.5%)
1	J	0.91	0/1235	1.06	4/1664 (0.2%)
1	K	0.97	1/1228 (0.1%)	1.09	5/1654 (0.3%)
1	L	0.92	1/1249 (0.1%)	1.07	7/1683 (0.4%)
All	All	0.94	11/14842 (0.1%)	1.08	59/19997 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	55	GLU	CG-CD	6.96	1.62	1.51
1	L	154	PRO	N-CD	-6.02	1.39	1.47
1	F	120	THR	CB-CG2	-5.71	1.33	1.52
1	B	156	GLU	CG-CD	5.59	1.60	1.51
1	F	156	GLU	CB-CG	5.52	1.62	1.52
1	B	156	GLU	CB-CG	5.50	1.62	1.52
1	K	120	THR	CB-CG2	-5.46	1.34	1.52
1	F	72	PHE	CE1-CZ	5.20	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	123	GLU	CG-CD	5.18	1.59	1.51
1	C	44	GLU	CG-CD	5.06	1.59	1.51
1	F	156	GLU	CG-CD	5.06	1.59	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	119	LEU	CA-CB-CG	8.38	134.57	115.30
1	A	119	LEU	CA-CB-CG	8.01	133.71	115.30
1	A	34	MET	CG-SD-CE	-7.97	87.45	100.20
1	L	155	LEU	O-C-N	-7.44	110.80	122.70
1	B	96	ASP	CB-CG-OD1	7.38	124.95	118.30
1	K	8	ASP	CB-CA-C	7.28	124.96	110.40
1	K	102	LEU	CA-CB-CG	7.28	132.04	115.30
1	H	8	ASP	CB-CA-C	7.05	124.51	110.40
1	F	65	LEU	CA-CB-CG	6.90	131.18	115.30
1	H	8	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	G	119	LEU	CA-CB-CG	6.75	130.82	115.30
1	I	65	LEU	CA-CB-CG	6.60	130.47	115.30
1	F	65	LEU	CB-CG-CD1	6.51	122.08	111.00
1	I	65	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	L	65	LEU	CA-CB-CG	6.41	130.05	115.30
1	C	65	LEU	CA-CB-CG	6.28	129.74	115.30
1	I	58	ASP	CB-CG-OD2	6.16	123.84	118.30
1	L	102	LEU	CA-CB-CG	6.12	129.37	115.30
1	J	132	LEU	CA-CB-CG	6.09	129.30	115.30
1	K	58	ASP	CB-CG-OD2	6.06	123.76	118.30
1	C	102	LEU	CA-CB-CG	6.05	129.22	115.30
1	E	65	LEU	CB-CG-CD1	6.00	121.20	111.00
1	J	102	LEU	CA-CB-CG	5.86	128.78	115.30
1	I	34	MET	CG-SD-CE	-5.85	90.84	100.20
1	G	65	LEU	CA-CB-CG	5.83	128.72	115.30
1	G	132	LEU	CB-CG-CD1	5.81	120.88	111.00
1	K	65	LEU	CB-CG-CD1	5.75	120.77	111.00
1	E	132	LEU	CB-CG-CD1	5.71	120.70	111.00
1	B	156	GLU	N-CA-CB	-5.68	100.37	110.60
1	E	65	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	99	MET	CG-SD-CE	-5.63	91.20	100.20
1	G	102	LEU	CA-CB-CG	5.62	128.23	115.30
1	B	48	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	H	58[A]	ASP	CB-CG-OD2	5.59	123.33	118.30
1	H	58[B]	ASP	CB-CG-OD2	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	8	ASP	CB-CG-OD1	5.59	123.33	118.30
1	H	8	ASP	CB-CG-OD1	5.52	123.27	118.30
1	J	65	LEU	CA-CB-CG	5.52	128.00	115.30
1	I	58	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	L	65	LEU	CB-CG-CD1	5.51	120.37	111.00
1	E	111	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	K	20	LEU	CB-CG-CD1	5.41	120.19	111.00
1	H	65	LEU	CB-CG-CD1	5.37	120.12	111.00
1	L	110	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	G	121	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	20	LEU	CA-CB-CG	5.29	127.48	115.30
1	D	65	LEU	CA-CB-CG	5.29	127.46	115.30
1	I	132	LEU	CB-CG-CD1	5.26	119.94	111.00
1	B	156	GLU	CA-CB-CG	5.24	124.93	113.40
1	D	102	LEU	CA-CB-CG	5.20	127.26	115.30
1	F	152	LYS	CD-CE-NZ	5.17	123.60	111.70
1	H	136	LYS	CD-CE-NZ	5.17	123.59	111.70
1	E	102	LEU	CA-CB-CG	5.17	127.18	115.30
1	C	132	LEU	CA-CB-CG	5.13	127.11	115.30
1	E	20	LEU	CA-CB-CG	5.12	127.09	115.30
1	L	132	LEU	CB-CG-CD1	5.10	119.67	111.00
1	I	13	LEU	CB-CG-CD1	5.02	119.53	111.00
1	L	101	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	20	LEU	CB-CG-CD1	5.00	119.50	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	K	8	ASP	CA

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	1210	0	1178	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1216	0	1183	29	0
1	C	1210	0	1178	12	0
1	D	1214	0	1178	13	0
1	E	1210	0	1178	11	0
1	F	1210	0	1178	23	0
1	G	1210	0	1178	11	0
1	H	1207	0	1169	23	0
1	I	1210	0	1178	16	0
1	J	1210	0	1178	20	0
1	K	1203	0	1169	21	0
1	L	1224	0	1189	17	0
2	A	7	0	0	0	0
2	B	14	0	0	1	0
2	C	13	0	0	0	0
2	D	17	0	0	0	0
2	E	16	0	0	0	0
2	F	8	0	0	0	0
2	G	11	0	0	0	0
2	H	25	0	0	0	0
2	I	11	0	0	0	0
2	J	17	0	0	0	0
2	K	9	0	0	0	0
2	L	14	0	0	0	0
All	All	14696	0	14134	174	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 6.

All (174) 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:54:GLY:O	1:D:58[A]:ASP:OD2	1.91	0.87
1:I:153:ALA:HB3	1:I:156:GLU:HG2	1.63	0.80
1:J:38:ASN:HB3	1:J:42:LEU:HD23	1.69	0.73
1:L:147:LYS:NZ	1:L:156:GLU:C	2.41	0.73
1:G:116:GLY:O	1:G:120:THR:HB	1.92	0.68
1:B:38:ASN:HD21	1:J:37:HIS:HB3	1.59	0.68
1:L:147:LYS:HZ1	1:L:156:GLU:C	1.97	0.67
1:F:116:GLY:O	1:F:120:THR:HB	1.94	0.67
1:B:37:HIS:HB3	1:F:38:ASN:HD21	1.61	0.66
1:A:94:THR:H	1:A:97:GLN:HG3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:THR:HG23	1:D:129:ASN:HB2	1.79	0.65
1:B:6:SER:HB3	2:B:2001:HOH:O	1.96	0.64
1:F:32:TRP:HB3	1:H:65:LEU:HD21	1.79	0.64
1:F:150:LEU:O	1:F:152:LYS:HE3	1.97	0.64
1:B:156:GLU:CG	1:B:156:GLU:O	2.45	0.63
1:F:34:MET:SD	1:F:95:MET:HB2	2.38	0.63
1:B:20:LEU:HD23	1:B:57:MET:HA	1.80	0.63
1:F:95:MET:C	1:F:95:MET:SD	2.77	0.63
1:J:120:THR:HG23	1:J:129:ASN:HB2	1.82	0.61
1:B:65:LEU:HD13	1:B:71:PRO:HD3	1.82	0.60
1:E:32:TRP:HB3	1:G:65:LEU:HD21	1.84	0.60
1:L:42:LEU:HD23	1:L:95:MET:SD	2.42	0.59
1:K:24:THR:HG23	1:K:50:TYR:CE2	2.38	0.59
1:D:38:ASN:HD21	1:I:37:HIS:HB3	1.67	0.58
1:B:116:GLY:O	1:B:120:THR:HB	2.03	0.58
1:L:94:THR:HG22	1:L:96:ASP:H	1.69	0.58
1:H:120:THR:HG23	1:H:129:ASN:HB2	1.87	0.57
1:I:30:ILE:O	1:I:34:MET:HB2	2.04	0.57
1:A:36:GLY:O	1:H:149:PHE:HA	2.05	0.56
1:K:120:THR:HG23	1:K:125:ASP:HB3	1.87	0.56
1:B:153:ALA:O	1:B:156:GLU:HB2	2.05	0.56
1:E:38:ASN:HB3	1:E:42:LEU:HD23	1.87	0.56
1:A:94:THR:N	1:A:97:GLN:HG3	2.21	0.55
1:C:24:THR:HG23	1:C:50:TYR:CE2	2.41	0.55
1:J:15:HIS:HE1	1:J:83:SER:OG	1.89	0.55
1:B:34:MET:HB2	1:B:95:MET:SD	2.46	0.55
1:C:116:GLY:O	1:C:120:THR:HG22	2.07	0.54
1:L:24:THR:HG23	1:L:50:TYR:CE2	2.42	0.54
1:L:116:GLY:O	1:L:120:THR:HB	2.07	0.54
1:K:74:THR:OG1	1:K:77:GLU:HG3	2.07	0.54
1:L:147:LYS:HZ3	1:L:156:GLU:C	2.11	0.54
1:H:24:THR:HG23	1:H:50:TYR:CE2	2.43	0.53
1:B:30:ILE:HG21	1:B:99:MET:CE	2.38	0.53
1:B:156:GLU:O	1:B:156:GLU:CD	2.46	0.53
1:J:51:SER:O	1:J:55:GLU:HG2	2.07	0.53
1:H:30:ILE:HG21	1:H:99:MET:CE	2.39	0.53
1:H:37:HIS:HB3	1:K:38:ASN:OD1	2.09	0.52
1:H:24:THR:HG23	1:H:50:TYR:HE2	1.74	0.52
1:I:32:TRP:HB3	1:K:65:LEU:HD21	1.90	0.52
1:J:153:ALA:HB3	1:J:156:GLU:HB2	1.92	0.52
1:F:74:THR:OG1	1:F:77:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:O	1:A:34:MET:HB2	2.10	0.52
1:A:32:TRP:HB3	1:C:65:LEU:HD21	1.92	0.52
1:F:62:GLU:OE1	1:K:141:LYS:HE2	2.09	0.52
1:I:73:SER:HB2	1:K:29:GLN:HB2	1.92	0.52
1:G:120:THR:HG21	1:G:129:ASN:HA	1.92	0.52
1:F:76:LYS:HZ1	1:H:88:PRO:HD3	1.74	0.51
1:E:29:GLN:HB2	1:G:73:SER:HB2	1.92	0.51
1:E:120:THR:HG21	1:E:129:ASN:HA	1.92	0.51
1:L:152:LYS:HB3	1:L:156:GLU:HG3	1.92	0.51
1:G:94:THR:HG22	1:G:96:ASP:H	1.76	0.51
1:F:76:LYS:HZ2	1:F:77:GLU:HG3	1.75	0.51
1:I:64:LEU:CD1	1:I:69:GLY:HA3	2.41	0.50
1:J:29:GLN:HB2	1:L:73:SER:HB2	1.93	0.50
1:E:116:GLY:O	1:E:120:THR:HB	2.12	0.50
1:A:20:LEU:HD21	1:A:113:TYR:OH	2.11	0.50
1:D:20:LEU:HB3	1:D:57:MET:HB2	1.94	0.50
1:K:8:ASP:HA	1:K:119:LEU:HD21	1.95	0.49
1:B:152:LYS:HD2	1:B:156:GLU:HG3	1.95	0.49
1:H:35:ARG:HB3	1:K:151:GLY:HA2	1.94	0.49
1:I:20:LEU:O	1:I:24:THR:HB	2.13	0.49
1:B:65:LEU:HD13	1:B:71:PRO:CD	2.42	0.48
1:E:20:LEU:HB3	1:E:57:MET:HB2	1.94	0.48
1:B:120:THR:HG21	1:B:129:ASN:HA	1.94	0.48
1:L:120:THR:HG23	1:L:129:ASN:HB2	1.95	0.48
1:A:65:LEU:O	1:E:154:PRO:HG2	2.13	0.48
1:C:65:LEU:O	1:H:154:PRO:HG2	2.12	0.48
1:A:154:PRO:HG2	1:I:65:LEU:O	2.14	0.48
1:L:120:THR:HG21	1:L:129:ASN:HA	1.96	0.48
1:G:120:THR:CG2	1:G:129:ASN:HA	2.44	0.48
1:G:120:THR:HG23	1:G:129:ASN:HB2	1.95	0.48
1:E:120:THR:CG2	1:E:129:ASN:HA	2.45	0.47
1:H:27:ILE:HD13	1:H:49:LEU:HB3	1.96	0.47
1:A:95:MET:HE2	1:A:96:ASP:HA	1.96	0.47
1:D:120:THR:HG21	1:D:129:ASN:HA	1.97	0.47
1:J:118:GLU:HB3	1:J:122:LYS:HE2	1.95	0.47
1:G:147:LYS:HD2	1:G:152:LYS:HG3	1.96	0.47
1:A:49:LEU:HD21	1:A:102:LEU:HD21	1.96	0.47
1:F:65:LEU:O	1:K:154:PRO:HG2	2.15	0.47
1:I:30:ILE:HG21	1:I:99:MET:CE	2.44	0.47
1:I:52:GLU:OE2	1:I:138:SER:OG	2.32	0.47
1:K:94:THR:HG22	1:K:96:ASP:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:GLU:OE2	1:D:138:SER:OG	2.29	0.46
1:H:65:LEU:HD13	1:H:71:PRO:CD	2.45	0.46
1:D:95:MET:SD	1:D:95:MET:C	2.94	0.46
1:J:20:LEU:HB3	1:J:57:MET:HB2	1.97	0.46
1:K:12:PHE:CZ	1:K:116:GLY:HA3	2.50	0.46
1:C:153:ALA:HB3	1:C:156:GLU:HG3	1.97	0.46
1:F:114:LYS:HE3	1:F:114:LYS:O	2.15	0.46
1:A:20:LEU:HB3	1:A:57:MET:HB2	1.98	0.46
1:B:37:HIS:HB3	1:F:38:ASN:ND2	2.29	0.46
1:J:128:THR:O	1:J:132:LEU:HD22	2.16	0.46
1:I:15:HIS:HE1	1:I:83:SER:OG	2.00	0.45
1:B:32:TRP:HB3	1:D:65:LEU:HD21	1.97	0.45
1:I:29:GLN:HB2	1:K:73:SER:HB2	1.99	0.45
1:I:153:ALA:H	1:I:156:GLU:HG3	1.81	0.45
1:A:94:THR:H	1:A:97:GLN:CG	2.30	0.45
1:A:86:GLU:CD	1:C:74:THR:HB	2.37	0.45
1:H:20:LEU:HD23	1:H:57:MET:HA	1.98	0.45
1:H:65:LEU:O	1:J:154:PRO:HG2	2.16	0.45
1:A:38:ASN:HD21	1:K:37:HIS:HB3	1.82	0.44
1:F:20:LEU:HD23	1:F:57:MET:HA	1.99	0.44
1:H:34:MET:HB2	1:H:95:MET:CE	2.47	0.44
1:I:153:ALA:HB3	1:I:156:GLU:CG	2.42	0.44
1:K:120:THR:HG21	1:K:129:ASN:N	2.32	0.44
1:B:154:PRO:HG3	1:L:65:LEU:O	2.17	0.44
1:D:27:ILE:HD13	1:D:49:LEU:HB3	1.99	0.44
1:D:154:PRO:HG2	1:K:65:LEU:O	2.16	0.44
1:L:154:PRO:O	1:L:155:LEU:HD23	2.17	0.44
1:G:24:THR:HG23	1:G:50:TYR:CE2	2.53	0.44
1:B:29:GLN:HB2	1:D:73:SER:HB2	1.98	0.44
1:J:65:LEU:HD13	1:J:71:PRO:HD2	2.00	0.44
1:K:94:THR:HG22	1:K:96:ASP:N	2.32	0.44
1:F:72:PHE:HD2	1:F:77:GLU:OE2	2.01	0.44
1:B:15:HIS:HE1	1:B:83:SER:OG	2.01	0.43
1:B:152:LYS:HD2	1:B:156:GLU:CG	2.49	0.43
1:L:65:LEU:HD13	1:L:71:PRO:CD	2.48	0.43
1:B:24:THR:HG23	1:B:50:TYR:CE2	2.54	0.43
1:J:30:ILE:HG21	1:J:99:MET:CE	2.49	0.43
1:J:96:ASP:O	1:J:100:GLU:HG2	2.18	0.43
1:C:28:HIS:CE1	1:C:50:TYR:CE2	3.07	0.43
1:G:128:THR:HG22	1:G:132:LEU:HD22	2.00	0.43
1:L:20:LEU:HD23	1:L:57:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:120:THR:CG2	1:L:129:ASN:HA	2.49	0.43
1:B:99:MET:O	1:B:103:VAL:HG23	2.19	0.43
1:J:75:LEU:HD22	1:L:22:VAL:HG22	2.01	0.43
1:D:144:TRP:HB2	1:K:66:ALA:HA	2.01	0.43
1:B:147:LYS:HE3	1:B:156:GLU:HB3	2.01	0.42
1:C:14:ASN:OD1	1:C:71:PRO:HA	2.18	0.42
1:C:76:LYS:O	1:C:80:GLU:HB2	2.19	0.42
1:B:30:ILE:HG21	1:B:99:MET:HE2	2.00	0.42
1:B:14:ASN:OD1	1:B:71:PRO:HA	2.20	0.42
1:B:38:ASN:ND2	1:J:37:HIS:HB3	2.30	0.42
1:A:58:ASP:O	1:A:62:GLU:HG3	2.19	0.42
1:E:34:MET:HB2	1:E:95:MET:CE	2.50	0.42
1:H:14:ASN:OD1	1:H:71:PRO:HA	2.20	0.42
1:I:64:LEU:HD12	1:I:69:GLY:HA3	2.02	0.42
1:E:20:LEU:O	1:E:24:THR:HB	2.19	0.42
1:B:120:THR:HG23	1:B:129:ASN:HB2	2.00	0.42
1:F:37:HIS:HE1	1:J:96:ASP:OD2	2.02	0.42
1:E:73:SER:OG	1:G:29:GLN:HG3	2.20	0.42
1:J:20:LEU:HD23	1:J:57:MET:HA	2.01	0.42
1:F:30:ILE:HG21	1:F:99:MET:HE1	2.02	0.42
1:H:65:LEU:HD13	1:H:71:PRO:HD3	2.01	0.41
1:J:116:GLY:HA2	1:J:119:LEU:HD23	2.02	0.41
1:H:84:VAL:HG13	1:H:105:THR:HG23	2.02	0.41
1:I:7:VAL:HB	1:I:11:GLU:HG3	2.01	0.41
1:B:65:LEU:HD21	1:D:32:TRP:HB3	2.01	0.41
1:C:94:THR:HB	1:C:97:GLN:H	1.85	0.41
1:C:38:ASN:O	1:C:42:LEU:HB2	2.21	0.41
1:F:65:LEU:HD21	1:H:32:TRP:HB3	2.01	0.41
1:J:26:LYS:HE3	1:J:105:THR:OG1	2.20	0.41
1:B:120:THR:CG2	1:B:129:ASN:HA	2.51	0.41
1:F:30:ILE:HG21	1:F:99:MET:CE	2.50	0.41
1:K:65:LEU:HD13	1:K:71:PRO:HD3	2.01	0.40
1:C:95:MET:HA	1:C:95:MET:CE	2.50	0.40
1:F:65:LEU:HD13	1:F:71:PRO:CD	2.51	0.40
1:H:9:THR:HG22	1:H:13:LEU:HD22	2.03	0.40
1:A:45:LYS:HE3	1:K:40:PHE:CD2	2.56	0.40
1:F:66:ALA:HB1	1:K:140:ASP:HB3	2.03	0.40
1:F:76:LYS:NZ	1:H:88:PRO:HD3	2.35	0.40
1:F:120:THR:HG22	1:F:129:ASN:HD22	1.84	0.40
1:H:94:THR:HG22	1:H:97:GLN:H	1.87	0.40
1:H:99:MET:SD	1:H:102:LEU:HD12	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	B	149/156 (96%)	148 (99%)	1 (1%)	0	100	100
1	C	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	D	149/156 (96%)	147 (99%)	2 (1%)	0	100	100
1	E	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
1	F	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	G	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	H	148/156 (95%)	146 (99%)	2 (1%)	0	100	100
1	I	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	J	148/156 (95%)	147 (99%)	1 (1%)	0	100	100
1	K	147/156 (94%)	145 (99%)	2 (1%)	0	100	100
1	L	150/156 (96%)	148 (99%)	2 (1%)	0	100	100
All	All	1779/1872 (95%)	1757 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	131/137 (96%)	120 (92%)	11 (8%)	11	21
1	B	132/137 (96%)	122 (92%)	10 (8%)	13	26
1	C	131/137 (96%)	121 (92%)	10 (8%)	13	26
1	D	132/137 (96%)	121 (92%)	11 (8%)	11	22
1	E	131/137 (96%)	120 (92%)	11 (8%)	11	21
1	F	131/137 (96%)	118 (90%)	13 (10%)	8	15
1	G	131/137 (96%)	120 (92%)	11 (8%)	11	21
1	H	131/137 (96%)	117 (89%)	14 (11%)	6	12
1	I	131/137 (96%)	119 (91%)	12 (9%)	9	17
1	J	131/137 (96%)	117 (89%)	14 (11%)	6	12
1	K	130/137 (95%)	120 (92%)	10 (8%)	13	25
1	L	133/137 (97%)	123 (92%)	10 (8%)	13	27
All	All	1575/1644 (96%)	1438 (91%)	137 (9%)	10	20

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	20	LEU
1	A	24	THR
1	A	42	LEU
1	A	45	LYS
1	A	95	MET
1	A	97	GLN
1	A	102	LEU
1	A	118	GLU
1	A	119	LEU
1	A	130	ASP
1	B	13	LEU
1	B	20	LEU
1	B	24	THR
1	B	65	LEU
1	B	79	LEU
1	B	94	THR
1	B	102	LEU
1	B	120	THR
1	B	132	LEU
1	B	141	LYS
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	20	LEU
1	C	24	THR
1	C	42	LEU
1	C	45	LYS
1	C	65	LEU
1	C	76	LYS
1	C	85	GLU
1	C	94	THR
1	C	132	LEU
1	D	13	LEU
1	D	20	LEU
1	D	24	THR
1	D	47	ASP
1	D	58[A]	ASP
1	D	58[B]	ASP
1	D	94	THR
1	D	96	ASP
1	D	102	LEU
1	D	120	THR
1	D	132	LEU
1	E	13	LEU
1	E	20	LEU
1	E	24	THR
1	E	45	LYS
1	E	55	GLU
1	E	65	LEU
1	E	94	THR
1	E	102	LEU
1	E	120	THR
1	E	121	ASP
1	E	132	LEU
1	F	13	LEU
1	F	20	LEU
1	F	24	THR
1	F	41	THR
1	F	42	LEU
1	F	65	LEU
1	F	76	LYS
1	F	95	MET
1	F	102	LEU
1	F	114	LYS
1	F	120	THR

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Mol	Chain	Res	Type
1	F	132	LEU
1	F	152	LYS
1	G	7	VAL
1	G	13	LEU
1	G	20	LEU
1	G	24	THR
1	G	42	LEU
1	G	55	GLU
1	G	65	LEU
1	G	102	LEU
1	G	120	THR
1	G	130	ASP
1	G	132	LEU
1	H	8	ASP
1	H	13	LEU
1	H	20	LEU
1	H	24	THR
1	H	49	LEU
1	H	55	GLU
1	H	65	LEU
1	H	80	GLU
1	H	94	THR
1	H	102	LEU
1	H	120	THR
1	H	130	ASP
1	H	131	MET
1	H	132	LEU
1	I	13	LEU
1	I	20	LEU
1	I	24	THR
1	I	42	LEU
1	I	45	LYS
1	I	49	LEU
1	I	65	LEU
1	I	96	ASP
1	I	102	LEU
1	I	118	GLU
1	I	130	ASP
1	I	132	LEU
1	J	13	LEU
1	J	20	LEU
1	J	24	THR

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Mol	Chain	Res	Type
1	J	41	THR
1	J	45	LYS
1	J	65	LEU
1	J	96	ASP
1	J	114	LYS
1	J	118	GLU
1	J	119	LEU
1	J	120	THR
1	J	122	LYS
1	J	132	LEU
1	J	152	LYS
1	K	20	LEU
1	K	24	THR
1	K	45	LYS
1	K	65	LEU
1	K	94	THR
1	K	100	GLU
1	K	103	VAL
1	K	122	LYS
1	K	123	GLU
1	K	132	LEU
1	L	13	LEU
1	L	20	LEU
1	L	24	THR
1	L	42	LEU
1	L	45	LYS
1	L	58	ASP
1	L	65	LEU
1	L	93	LYS
1	L	120	THR
1	L	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	29	GLN
1	A	38	ASN
1	B	15	HIS
1	B	29	GLN
1	B	38	ASN
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	81	ASN
1	B	97	GLN
1	B	129	ASN
1	C	15	HIS
1	C	29	GLN
1	C	38	ASN
1	C	81	ASN
1	D	29	GLN
1	D	38	ASN
1	D	81	ASN
1	E	15	HIS
1	F	28	HIS
1	F	29	GLN
1	F	37	HIS
1	F	38	ASN
1	F	129	ASN
1	G	29	GLN
1	G	81	ASN
1	G	129	ASN
1	H	29	GLN
1	H	37	HIS
1	H	38	ASN
1	I	15	HIS
1	I	29	GLN
1	I	129	ASN
1	J	15	HIS
1	J	29	GLN
1	J	129	ASN
1	K	15	HIS
1	K	129	ASN
1	L	15	HIS
1	L	28	HIS
1	L	29	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 ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	150/156 (96%)	-0.31	4 (2%)	54	48	10, 18, 33, 41	0
1	B	151/156 (96%)	-0.27	2 (1%)	77	73	12, 18, 33, 42	0
1	C	150/156 (96%)	-0.29	0	100	100	12, 18, 33, 39	0
1	D	150/156 (96%)	-0.27	3 (2%)	65	60	12, 18, 33, 39	0
1	E	150/156 (96%)	-0.31	1 (0%)	87	86	12, 18, 32, 41	0
1	F	150/156 (96%)	-0.31	1 (0%)	87	86	11, 18, 32, 43	0
1	G	150/156 (96%)	-0.38	0	100	100	10, 18, 32, 40	0
1	H	149/156 (95%)	-0.37	0	100	100	10, 18, 31, 40	0
1	I	150/156 (96%)	-0.22	3 (2%)	65	60	10, 18, 32, 42	0
1	J	150/156 (96%)	-0.34	0	100	100	10, 18, 32, 40	0
1	K	149/156 (95%)	-0.33	1 (0%)	87	86	11, 18, 31, 40	0
1	L	152/156 (97%)	-0.30	2 (1%)	77	73	11, 18, 34, 43	0
All	All	1801/1872 (96%)	-0.31	17 (0%)	84	82	10, 18, 33, 43	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	7	VAL	3.7
1	F	156	GLU	3.6
1	B	156	GLU	3.4
1	E	156	GLU	3.4
1	A	156	GLU	3.2
1	L	156	GLU	2.9
1	A	91	LYS	2.9
1	A	92	PRO	2.7
1	B	155	LEU	2.7
1	I	156	GLU	2.6
1	A	90	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	96	ASP	2.5
1	D	155	LEU	2.2
1	I	91	LYS	2.1
1	L	91	LYS	2.1
1	D	7	VAL	2.1
1	K	90	THR	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.