



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 06:44 AM JST

PDB ID : 7FDL
Title : Crystal structure of transcription factor WER in complex with EGL3
Authors : Luo, Q.; Wang, B.
Deposited on : 2021-07-17
Resolution : 2.90 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

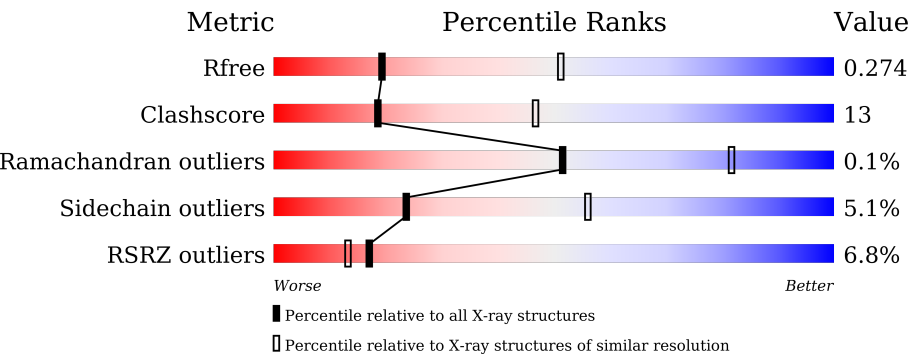
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	198	<div><div></div><div><div></div><div>63%</div><div>25%</div><div>•</div><div>12%</div></div></div>
1	C	198	<div><div></div><div><div></div><div>66%</div><div>19%</div><div>•</div><div>14%</div></div></div>
1	E	198	<div><div>13%</div><div><div></div><div>47%</div><div>14%</div><div>•</div><div>37%</div></div></div>
1	G	198	<div><div>4%</div><div><div></div><div>59%</div><div>22%</div><div>•</div><div>18%</div></div></div>
1	I	198	<div><div>2%</div><div><div></div><div>60%</div><div>25%</div><div>•</div><div>15%</div></div></div>
1	K	198	<div><div>6%</div><div><div></div><div>49%</div><div>19%</div><div>•</div><div>31%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	54	<div><div></div><div>56%26%17%</div></div>
2	D	54	<div><div></div><div>63%20%15%</div></div>
2	F	54	<div><div></div><div>28%67%6%26%</div></div>
2	H	54	<div><div></div><div>54%30%17%</div></div>
2	J	54	<div><div></div><div>11%50%28%20%</div></div>
2	L	54	<div><div></div><div>13%24%74%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8866 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 Transcription factor EGL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1334	857	218	254	5			
1	C	171	Total	C	N	O	S	0	0	0
			1319	847	210	257	5			
1	E	125	Total	C	N	O	S	0	0	0
			925	595	149	176	5			
1	G	162	Total	C	N	O	S	0	0	0
			1196	773	190	228	5			
1	I	169	Total	C	N	O	S	0	0	0
			1296	827	209	255	5			
1	K	136	Total	C	N	O	S	0	0	0
			938	603	155	176	4			

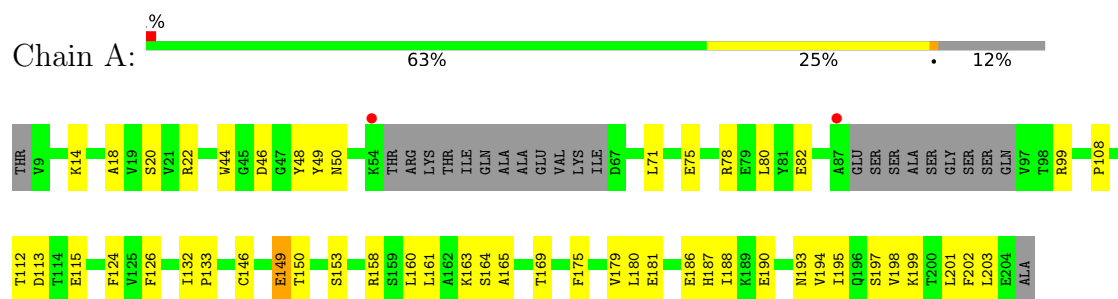
- Molecule 2 is a protein called Transcription factor WER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	0	0	0
			376	237	72	67			
2	D	46	Total	C	N	O	0	0	0
			385	243	74	68			
2	F	40	Total	C	N	O	0	0	0
			271	171	50	50			
2	H	45	Total	C	N	O	0	0	0
			379	240	72	67			
2	J	43	Total	C	N	O	0	0	0
			351	224	67	60			
2	L	14	Total	C	N	O	0	0	0
			96	59	17	20			

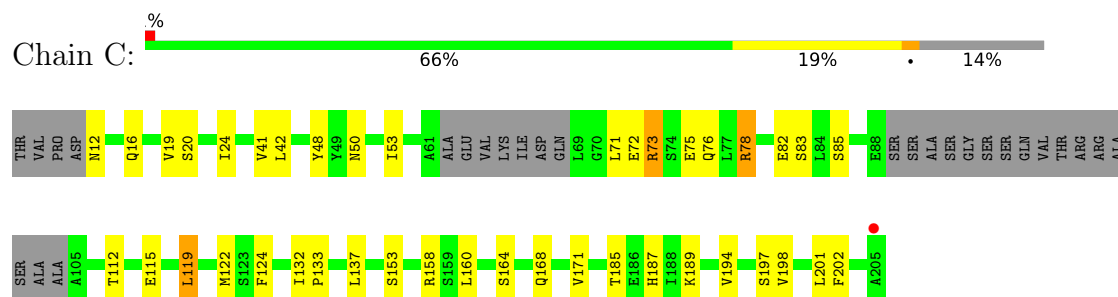
3 Residue-property plots [i](#)

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.

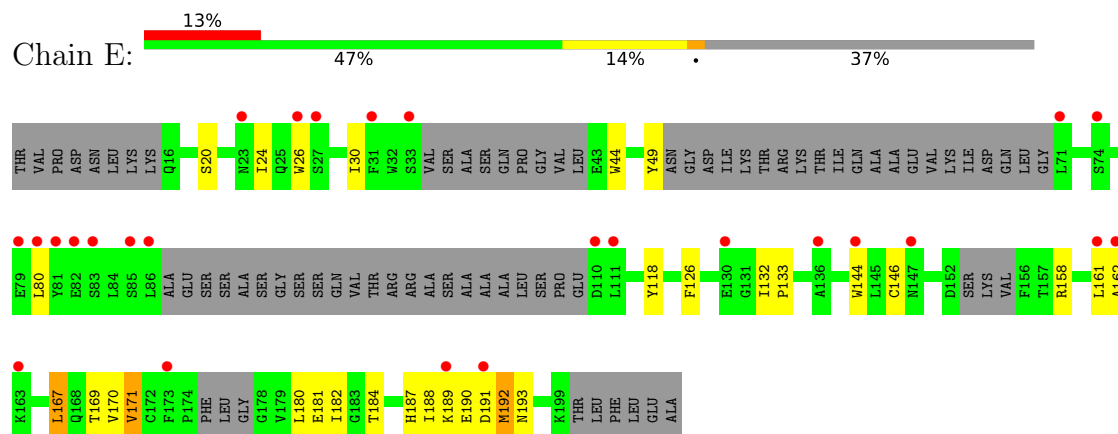
• Molecule 1: Transcription factor EGL1



• Molecule 1: Transcription factor EGL1

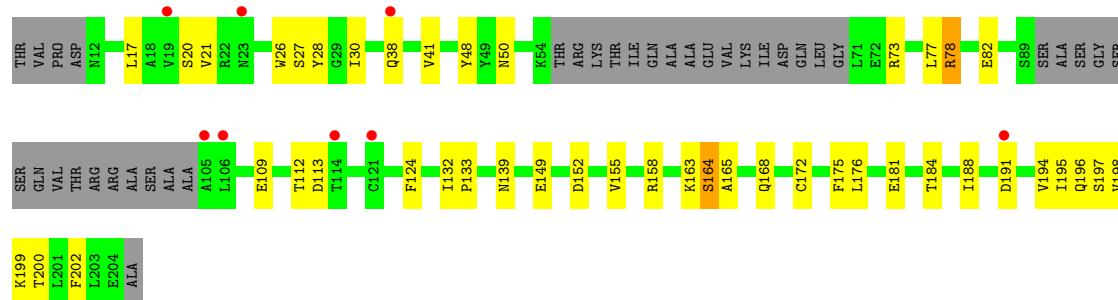


• Molecule 1: Transcription factor EGL1

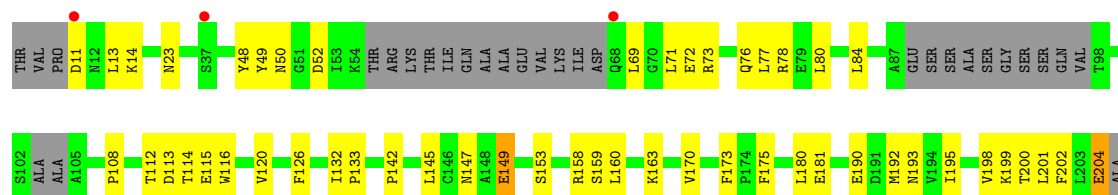


• Molecule 1: Transcription factor EGL1

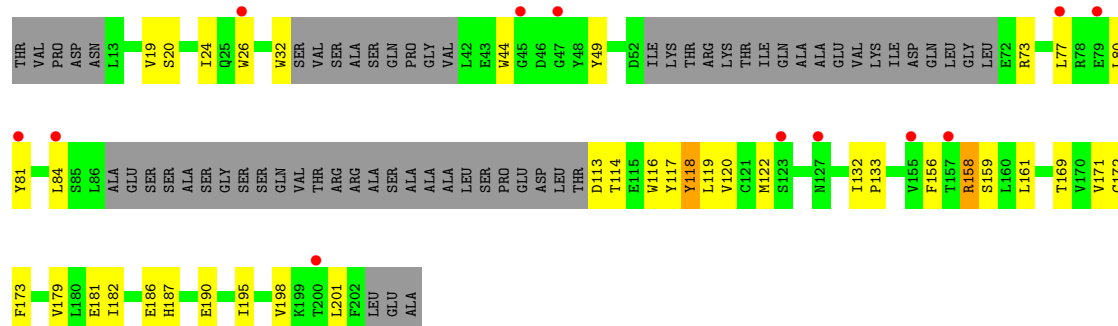




- Molecule 1: Transcription factor EGL1



- Molecule 1: Transcription factor EGL1



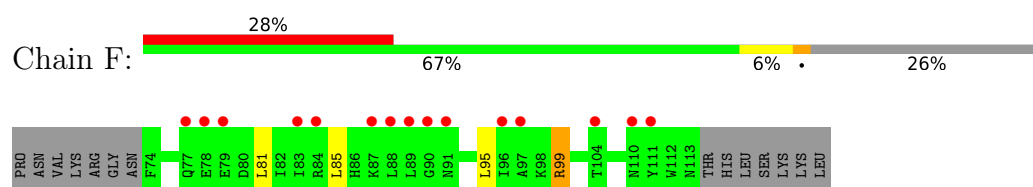
- Molecule 2: Transcription factor WER



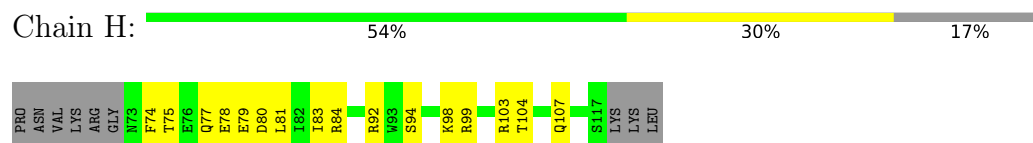
- Molecule 2: Transcription factor WER



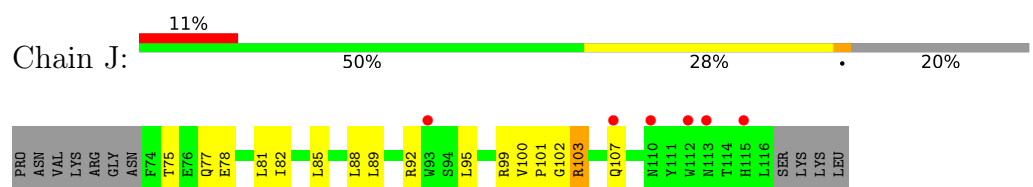
- Molecule 2: Transcription factor WER



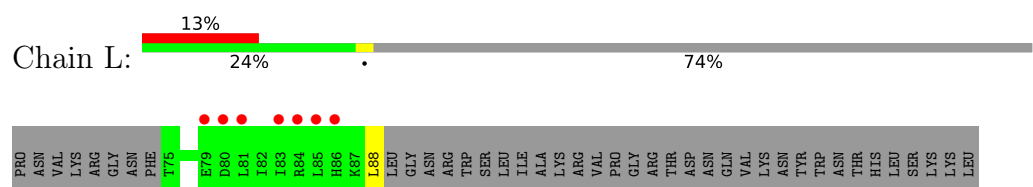
- Molecule 2: Transcription factor WER



- Molecule 2: Transcription factor WER



- Molecule 2: Transcription factor WER



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.91Å 193.39Å 224.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.90 29.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.9 (29.91-2.90) 84.9 (29.91-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.90Å)	Xtriage
Refinement program	REFMAC 7.0.076	Depositor
R, R_{free}	0.254 , 0.298 0.271 , 0.274	Depositor DCC
R_{free} test set	1563 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8866	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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	A	0.53	0/1361	0.66	0/1850
1	C	0.53	0/1345	0.62	0/1825
1	E	0.44	0/944	0.59	0/1284
1	G	0.45	0/1222	0.61	0/1667
1	I	0.43	0/1321	0.64	0/1794
1	K	0.43	0/955	0.62	0/1306
2	B	0.58	0/384	0.61	0/519
2	D	0.35	0/393	0.56	0/531
2	F	0.27	0/276	0.55	0/380
2	H	0.36	0/387	0.66	0/523
2	J	0.44	0/358	0.78	0/486
2	L	0.33	0/95	0.64	0/128
All	All	0.46	0/9041	0.63	0/12293

There are no bond length outliers.

There are no bond angle outliers.

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	1334	0	1291	39	0
1	C	1319	0	1283	23	0
1	E	925	0	807	33	0
1	G	1196	0	1105	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1296	0	1230	36	0
1	K	938	0	810	28	0
2	B	376	0	367	12	0
2	D	385	0	380	9	0
2	F	271	0	208	2	0
2	H	379	0	376	14	0
2	J	351	0	345	17	0
2	L	96	0	75	2	0
All	All	8866	0	8277	226	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 13.

All (226) 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:A:193:ASN:OD1	2:J:75:THR:HG23	1.44	1.18
1:G:191:ASP:O	1:G:194:VAL:HG12	1.52	1.09
2:D:99:ARG:HH21	2:D:99:ARG:HG3	1.29	0.96
2:B:75:THR:HB	2:B:78:GLU:HG3	1.53	0.91
1:E:189:LYS:NZ	1:G:168:GLN:CB	2.36	0.89
2:H:75:THR:HG22	2:H:78:GLU:HG2	1.56	0.87
1:E:189:LYS:HZ1	1:G:168:GLN:CB	1.89	0.85
1:E:192:MET:HE2	1:E:192:MET:HA	1.61	0.82
2:B:92:ARG:HD2	2:B:95:LEU:HD12	1.63	0.80
1:I:112:THR:HG22	1:I:115:GLU:HG3	1.65	0.77
2:D:99:ARG:HG3	2:D:99:ARG:NH2	1.95	0.77
1:K:84:LEU:HB3	2:L:88:LEU:HD12	1.68	0.76
1:A:78:ARG:O	1:A:82:GLU:HG3	1.87	0.75
1:G:195:ILE:O	1:G:199:LYS:HG3	1.87	0.74
1:A:193:ASN:OD1	2:J:75:THR:CG2	2.30	0.74
1:A:169:THR:HG21	1:A:188:ILE:H	1.55	0.72
1:I:73:ARG:O	1:I:77:LEU:HD12	1.90	0.72
1:E:162:ALA:HA	1:E:167:LEU:HD21	1.72	0.72
2:J:78:GLU:O	2:J:82:ILE:HD12	1.92	0.70
1:I:80:LEU:O	1:I:84:LEU:HD12	1.91	0.70
1:C:132:ILE:HG13	1:C:133:PRO:HD3	1.73	0.70
2:H:104:THR:HG23	2:H:107:GLN:HE21	1.57	0.70
1:I:132:ILE:HG23	1:I:133:PRO:HD3	1.74	0.69
1:I:77:LEU:HD21	1:I:115:GLU:HB3	1.73	0.69
1:I:160:LEU:HD11	2:J:101:PRO:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:THR:HG22	2:B:77:GLN:H	1.58	0.68
2:H:74:PHE:HB3	2:H:78:GLU:HG3	1.73	0.68
1:E:169:THR:HB	1:E:184:THR:HG22	1.75	0.68
2:F:81:LEU:O	2:F:85:LEU:HD12	1.94	0.67
2:J:88:LEU:HB2	2:J:89:LEU:HD12	1.77	0.66
1:G:112:THR:HG22	1:G:113:ASP:H	1.60	0.66
2:H:80:ASP:O	2:H:84:ARG:HG3	1.95	0.66
1:E:44:TRP:HH2	1:E:118:TYR:HE1	1.45	0.65
1:E:189:LYS:HZ2	1:G:168:GLN:CB	2.09	0.65
1:K:44:TRP:NE1	1:K:122:MET:HA	2.13	0.63
2:J:85:LEU:HB3	2:J:89:LEU:HD13	1.80	0.63
1:A:175:PHE:HD2	1:A:180:LEU:HD13	1.62	0.62
1:K:81:TYR:HD1	1:K:119:LEU:HD21	1.64	0.62
2:F:95:LEU:O	2:F:99:ARG:HG2	2.00	0.62
1:E:188:ILE:O	1:E:188:ILE:HD12	1.99	0.62
1:I:142:PRO:HB3	1:I:173:PHE:HB3	1.81	0.62
1:G:48:TYR:CE2	1:G:50:ASN:HB2	2.35	0.62
1:C:71:LEU:O	1:C:75:GLU:HG3	1.99	0.61
1:K:32:TRP:HB2	1:K:179:VAL:HG22	1.81	0.61
1:A:18:ALA:O	1:A:22:ARG:HG3	2.00	0.61
1:K:116:TRP:O	1:K:120:VAL:HG23	2.01	0.61
2:H:75:THR:HG23	2:H:77:GLN:H	1.65	0.61
1:K:133:PRO:HB3	1:K:179:VAL:HG21	1.83	0.61
1:A:132:ILE:HG13	1:A:133:PRO:HD3	1.83	0.61
1:A:187:HIS:O	1:A:188:ILE:HD13	2.00	0.61
2:J:81:LEU:O	2:J:85:LEU:HD12	2.01	0.60
1:G:27:SER:H	1:G:184:THR:HG22	1.65	0.60
1:E:192:MET:HA	1:E:192:MET:CE	2.29	0.60
1:E:192:MET:HG3	1:E:192:MET:O	2.00	0.60
1:I:72:GLU:O	1:I:76:GLN:HG2	2.02	0.59
1:G:152:ASP:HB3	1:G:155:VAL:HG12	1.84	0.59
1:K:49:TYR:HB2	1:K:118:TYR:CE2	2.37	0.59
1:A:198:VAL:O	1:A:202:PHE:HB2	2.03	0.59
2:H:94:SER:O	2:H:98:LYS:HG2	2.03	0.59
1:G:26:TRP:CE2	1:G:188:ILE:HD12	2.37	0.59
1:K:49:TYR:HB2	1:K:118:TYR:HE2	1.68	0.59
2:H:80:ASP:OD1	2:H:84:ARG:NH1	2.36	0.58
1:G:78:ARG:NH2	1:G:82:GLU:OE1	2.36	0.58
1:C:16:GLN:HA	1:C:19:VAL:HG22	1.86	0.58
2:J:95:LEU:O	2:J:99:ARG:HG2	2.04	0.57
1:C:72:GLU:O	1:C:76:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:100:VAL:HG12	2:J:103:ARG:HG2	1.87	0.57
1:I:69:LEU:HB2	1:I:71:LEU:HD23	1.85	0.57
1:A:20:SER:HB3	1:A:198:VAL:HG13	1.86	0.57
1:I:84:LEU:HB3	2:J:88:LEU:O	2.05	0.57
1:C:194:VAL:O	1:C:198:VAL:HG23	2.03	0.56
1:E:158:ARG:HB3	1:E:161:LEU:HB3	1.86	0.56
1:G:194:VAL:O	1:G:198:VAL:HG13	2.04	0.56
1:A:113:ASP:HB3	1:A:165:ALA:HA	1.88	0.56
1:A:160:LEU:HD11	2:B:101:PRO:HD2	1.86	0.56
2:B:75:THR:CB	2:B:78:GLU:HG3	2.32	0.56
1:I:175:PHE:CE1	1:I:199:LYS:HD3	2.41	0.56
2:D:94:SER:O	2:D:98:LYS:HG3	2.06	0.55
2:D:99:ARG:HH21	2:D:99:ARG:CG	2.08	0.55
1:E:132:ILE:HG13	1:E:133:PRO:HD3	1.88	0.55
1:G:198:VAL:O	1:G:202:PHE:HB2	2.06	0.55
2:B:102:GLY:C	2:B:103:ARG:HD3	2.27	0.55
1:G:27:SER:OG	1:G:184:THR:HA	2.05	0.55
1:E:49:TYR:HB2	1:E:118:TYR:CD2	2.41	0.55
1:I:48:TYR:CE2	1:I:50:ASN:HB2	2.42	0.55
1:K:81:TYR:CD1	1:K:119:LEU:HD21	2.42	0.55
1:G:196:GLN:O	1:G:200:THR:HG23	2.07	0.54
1:C:12:ASN:O	1:C:16:GLN:HG2	2.07	0.54
1:A:187:HIS:C	1:A:188:ILE:HD13	2.28	0.54
1:I:113:ASP:OD1	2:J:99:ARG:NH1	2.32	0.54
1:G:113:ASP:HB3	1:G:165:ALA:HA	1.89	0.54
1:I:49:TYR:CZ	1:I:115:GLU:HG2	2.43	0.53
1:A:71:LEU:O	1:A:75:GLU:HG3	2.07	0.53
1:C:198:VAL:O	1:C:202:PHE:HB2	2.08	0.53
1:G:149:GLU:HB3	1:G:163:LYS:HB2	1.90	0.53
1:G:73:ARG:O	1:G:77:LEU:HD12	2.09	0.53
1:A:194:VAL:O	1:A:198:VAL:HG23	2.08	0.53
2:B:80:ASP:OD2	2:B:84:ARG:NH1	2.40	0.53
1:C:20:SER:HB2	1:C:198:VAL:HG13	1.91	0.53
1:C:42:LEU:HD11	1:C:137:LEU:HD22	1.91	0.52
1:G:26:TRP:NE1	1:G:188:ILE:HD12	2.24	0.52
1:E:49:TYR:HB2	1:E:118:TYR:CE2	2.45	0.52
1:G:191:ASP:HB3	1:G:194:VAL:HG12	1.90	0.52
1:A:44:TRP:CZ3	1:A:46:ASP:HA	2.45	0.52
1:C:78:ARG:O	1:C:82:GLU:HG3	2.09	0.52
2:J:100:VAL:CG1	2:J:103:ARG:HG2	2.38	0.52
1:A:197:SER:O	1:A:201:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:NH1	1:A:181:GLU:OE1	2.42	0.52
1:G:175:PHE:HE1	1:G:176:LEU:HD12	1.74	0.52
1:E:192:MET:CE	1:E:192:MET:CA	2.86	0.52
1:A:48:TYR:HE2	1:A:50:ASN:HB2	1.75	0.51
1:A:49:TYR:CZ	1:A:115:GLU:HG2	2.45	0.51
1:K:117:TYR:HA	1:K:161:LEU:HD21	1.91	0.51
1:G:112:THR:HG22	1:G:113:ASP:N	2.26	0.51
1:E:188:ILE:HD12	1:E:188:ILE:C	2.30	0.51
2:H:79:GLU:O	2:H:83:ILE:HG13	2.10	0.51
1:A:149:GLU:HB3	1:A:163:LYS:HA	1.93	0.51
1:G:172:CYS:SG	1:G:181:GLU:HB2	2.51	0.51
2:D:93:TRP:HH2	2:D:112:TRP:CD1	2.29	0.50
1:K:158:ARG:NH1	1:K:181:GLU:OE1	2.45	0.50
1:I:153:SER:OG	2:J:77:GLN:HG3	2.12	0.50
1:C:20:SER:O	1:C:24:ILE:HG12	2.12	0.50
1:C:119:LEU:HA	1:C:122:MET:CE	2.42	0.50
1:E:170:VAL:HG23	1:E:170:VAL:O	2.12	0.49
1:A:186:GLU:HB2	1:A:188:ILE:HD11	1.95	0.49
1:A:175:PHE:CD2	1:A:180:LEU:HD13	2.44	0.49
2:B:95:LEU:O	2:B:99:ARG:HG2	2.13	0.49
1:I:113:ASP:HB3	2:J:99:ARG:HH22	1.76	0.49
1:A:124:PHE:HA	2:B:84:ARG:HH21	1.78	0.49
1:K:26:TRP:CZ3	1:K:182:ILE:HD12	2.48	0.49
1:C:119:LEU:HA	1:C:122:MET:HE3	1.94	0.48
1:E:171:VAL:HG13	1:E:182:ILE:HG13	1.94	0.48
1:C:187:HIS:HE1	1:I:147:ASN:HD21	1.61	0.48
1:A:48:TYR:CE2	1:A:50:ASN:HB2	2.48	0.48
1:E:169:THR:HG21	1:E:188:ILE:CG1	2.43	0.48
1:I:112:THR:HG23	1:I:114:THR:H	1.77	0.48
1:K:156:PHE:CE2	1:K:159:SER:HA	2.48	0.47
1:I:13:LEU:HD12	1:I:202:PHE:HZ	1.79	0.47
1:K:49:TYR:HE2	1:K:114:THR:HG1	1.61	0.47
1:E:190:GLU:HG2	1:E:190:GLU:O	2.14	0.47
1:I:200:THR:O	1:I:204:GLU:HG3	2.13	0.47
1:K:173:PHE:CZ	1:K:198:VAL:HG21	2.49	0.47
1:A:190:GLU:O	1:A:190:GLU:HG2	2.15	0.47
1:A:150:THR:HG21	1:K:190:GLU:HB3	1.97	0.47
1:G:199:LYS:HA	1:G:202:PHE:HB2	1.96	0.47
1:A:195:ILE:HG22	1:A:199:LYS:HE3	1.98	0.46
1:E:30:ILE:O	1:E:180:LEU:HD12	2.16	0.46
1:I:158:ARG:NH1	1:I:181:GLU:OE2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:VAL:O	1:I:202:PHE:HB2	2.15	0.46
1:K:49:TYR:HD2	1:K:118:TYR:HD2	1.63	0.46
2:D:80:ASP:OD1	2:D:84:ARG:NH2	2.49	0.46
1:G:195:ILE:O	1:G:198:VAL:HG22	2.14	0.46
1:I:69:LEU:CB	1:I:71:LEU:HD23	2.45	0.46
1:I:108:PRO:HG2	2:J:92:ARG:HH21	1.81	0.46
1:E:191:ASP:C	1:E:193:ASN:N	2.67	0.45
2:H:75:THR:HG23	2:H:77:GLN:N	2.30	0.45
2:H:103:ARG:HA	2:H:103:ARG:HD3	1.83	0.45
1:A:49:TYR:CE2	1:A:115:GLU:HG2	2.52	0.45
1:K:19:VAL:HG22	1:K:201:LEU:HD21	1.98	0.45
1:K:84:LEU:C	2:L:88:LEU:HD12	2.36	0.45
1:C:112:THR:OG1	1:C:115:GLU:HG3	2.16	0.45
2:B:79:GLU:O	2:B:83:ILE:HG13	2.17	0.45
1:A:161:LEU:HD13	2:B:81:LEU:HD11	1.98	0.45
1:G:132:ILE:CG1	1:G:133:PRO:HD3	2.47	0.45
1:G:27:SER:N	1:G:184:THR:HG22	2.32	0.44
1:C:82:GLU:HA	1:C:85:SER:OG	2.16	0.44
1:K:44:TRP:HH2	1:K:118:TYR:HE1	1.64	0.44
1:E:169:THR:HG21	1:E:188:ILE:HG13	1.98	0.44
1:K:20:SER:HA	1:K:201:LEU:HD22	2.00	0.44
1:K:24:ILE:HG22	1:K:26:TRP:CD1	2.52	0.44
1:E:181:GLU:HG3	1:E:182:ILE:N	2.31	0.44
1:A:44:TRP:CH2	1:A:46:ASP:HA	2.53	0.44
1:C:160:LEU:HD11	2:D:101:PRO:HD2	1.99	0.44
1:K:169:THR:HG23	1:K:186:GLU:O	2.17	0.44
1:E:146:CYS:HB2	1:E:187:HIS:HE1	1.83	0.44
1:G:28:TYR:CD2	1:G:30:ILE:HG13	2.53	0.43
1:I:116:TRP:CH2	2:J:89:LEU:HD21	2.52	0.43
1:K:132:ILE:HB	1:K:133:PRO:HD3	2.00	0.43
1:A:132:ILE:CG1	1:A:133:PRO:HD3	2.48	0.43
1:A:126:PHE:CE2	1:A:133:PRO:HG2	2.54	0.43
1:C:53:ILE:HG21	1:C:73:ARG:HD2	2.00	0.43
1:E:192:MET:HB2	1:E:192:MET:HE3	1.64	0.43
1:I:112:THR:HG23	1:I:114:THR:N	2.34	0.43
1:E:191:ASP:OD2	1:E:191:ASP:N	2.51	0.43
1:I:132:ILE:CG2	1:I:133:PRO:HD3	2.47	0.43
1:E:20:SER:O	1:E:24:ILE:HG13	2.18	0.43
1:A:199:LYS:O	1:A:203:LEU:HD12	2.19	0.43
1:C:48:TYR:CE2	1:C:50:ASN:HB2	2.53	0.43
2:J:102:GLY:C	2:J:103:ARG:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:PHE:CZ	1:G:158:ARG:HG2	2.54	0.43
2:H:81:LEU:HD21	2:H:99:ARG:O	2.19	0.43
1:C:168:GLN:HG3	1:C:185:THR:O	2.17	0.43
1:I:149:GLU:HB3	1:I:163:LYS:HA	2.01	0.42
1:C:124:PHE:CZ	1:C:158:ARG:HG2	2.55	0.42
1:G:26:TRP:CZ2	1:G:188:ILE:HD12	2.55	0.42
1:I:11:ASP:HA	1:I:14:LYS:HG3	2.02	0.42
1:I:195:ILE:O	1:I:199:LYS:HG3	2.19	0.42
1:G:139:ASN:O	1:I:199:LYS:NZ	2.45	0.42
1:E:24:ILE:HD13	1:E:26:TRP:CG	2.54	0.42
1:G:38:GLN:O	1:G:41:VAL:HG12	2.20	0.42
1:G:164:SER:OG	2:H:99:ARG:NH2	2.45	0.42
1:C:197:SER:O	1:C:201:LEU:HG	2.20	0.42
1:E:132:ILE:N	1:E:133:PRO:CD	2.83	0.42
1:K:171:VAL:HB	1:K:182:ILE:HD11	2.02	0.41
2:D:75:THR:O	2:D:79:GLU:HG3	2.20	0.41
1:G:191:ASP:HB3	1:G:194:VAL:CG1	2.50	0.41
1:G:194:VAL:HA	1:G:197:SER:HB3	2.01	0.41
1:A:195:ILE:O	1:A:199:LYS:HG3	2.21	0.41
1:I:145:LEU:HB3	1:I:170:VAL:O	2.21	0.41
1:C:153:SER:OG	2:D:77:GLN:HG3	2.20	0.41
1:I:149:GLU:HB3	1:I:163:LYS:HB2	2.03	0.41
1:A:80:LEU:HD11	1:A:108:PRO:HD3	2.02	0.41
1:A:133:PRO:HA	1:A:179:VAL:HG11	2.03	0.41
1:A:187:HIS:CG	1:K:187:HIS:CD2	3.09	0.41
1:I:126:PHE:CE1	1:I:133:PRO:HG2	2.55	0.41
1:K:195:ILE:O	1:K:198:VAL:HG22	2.21	0.41
1:E:192:MET:HE2	1:E:192:MET:CA	2.38	0.40
1:G:17:LEU:O	1:G:21:VAL:HG22	2.20	0.40
1:K:119:LEU:C	1:K:119:LEU:HD23	2.41	0.40
1:I:116:TRP:O	1:I:120:VAL:HG23	2.21	0.40
1:E:126:PHE:CD1	1:E:133:PRO:HG2	2.56	0.40
1:E:132:ILE:CG1	1:E:133:PRO:HD3	2.50	0.40
2:H:78:GLU:OE1	2:H:103:ARG:NH2	2.54	0.40
1:I:23:ASN:OD1	1:I:201:LEU:HD11	2.21	0.40
1:A:124:PHE:HA	2:B:84:ARG:NH2	2.37	0.40
1:G:109:GLU:OE2	2:H:92:ARG:NH2	2.54	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	169/198 (85%)	156 (92%)	13 (8%)	0	100	100
1	C	165/198 (83%)	157 (95%)	8 (5%)	0	100	100
1	E	113/198 (57%)	101 (89%)	12 (11%)	0	100	100
1	G	156/198 (79%)	146 (94%)	10 (6%)	0	100	100
1	I	161/198 (81%)	148 (92%)	12 (8%)	1 (1%)	25	58
1	K	128/198 (65%)	115 (90%)	13 (10%)	0	100	100
2	B	43/54 (80%)	41 (95%)	2 (5%)	0	100	100
2	D	44/54 (82%)	42 (96%)	2 (4%)	0	100	100
2	F	38/54 (70%)	35 (92%)	3 (8%)	0	100	100
2	H	43/54 (80%)	40 (93%)	3 (7%)	0	100	100
2	J	41/54 (76%)	38 (93%)	3 (7%)	0	100	100
2	L	12/54 (22%)	12 (100%)	0	0	100	100
All	All	1113/1512 (74%)	1031 (93%)	81 (7%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	190	GLU

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	140/167 (84%)	133 (95%)	7 (5%)	24	57
1	C	142/167 (85%)	134 (94%)	8 (6%)	21	52
1	E	87/167 (52%)	82 (94%)	5 (6%)	20	51
1	G	119/167 (71%)	116 (98%)	3 (2%)	47	78
1	I	138/167 (83%)	130 (94%)	8 (6%)	20	50
1	K	81/167 (48%)	74 (91%)	7 (9%)	10	30
2	B	40/50 (80%)	38 (95%)	2 (5%)	24	57
2	D	41/50 (82%)	39 (95%)	2 (5%)	25	57
2	F	19/50 (38%)	18 (95%)	1 (5%)	22	54
2	H	41/50 (82%)	41 (100%)	0	100	100
2	J	36/50 (72%)	34 (94%)	2 (6%)	21	52
2	L	7/50 (14%)	7 (100%)	0	100	100
All	All	891/1302 (68%)	846 (95%)	45 (5%)	24	56

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	99	ARG
1	A	112	THR
1	A	146	CYS
1	A	149	GLU
1	A	153	SER
1	A	164	SER
2	B	76	GLU
2	B	77	GLN
1	C	41	VAL
1	C	73	ARG
1	C	78	ARG
1	C	83	SER
1	C	119	LEU
1	C	164	SER
1	C	171	VAL
1	C	189	LYS
2	D	99	ARG
2	D	104	THR
1	E	80	LEU
1	E	144	TRP
1	E	167	LEU

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Mol	Chain	Res	Type
1	E	171	VAL
1	E	192	MET
2	F	99	ARG
1	G	20	SER
1	G	78	ARG
1	G	164	SER
1	I	52	ASP
1	I	78	ARG
1	I	149	GLU
1	I	159	SER
1	I	180	LEU
1	I	192	MET
1	I	193	ASN
1	I	204	GLU
2	J	103	ARG
2	J	107	GLN
1	K	73	ARG
1	K	77	LEU
1	K	80	LEU
1	K	113	ASP
1	K	118	TYR
1	K	158	ARG
1	K	172	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	76	GLN
1	C	76	GLN
1	C	187	HIS
1	C	196	GLN
1	E	187	HIS
2	H	86	HIS
2	H	107	GLN
1	I	12	ASN
1	I	147	ASN

5.3.3 RNA ⓘ

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	175/198 (88%)	-0.14	2 (1%) 80 80	32, 46, 76, 92	0
1	C	171/198 (86%)	-0.35	1 (0%) 89 89	20, 33, 71, 101	0
1	E	125/198 (63%)	1.10	26 (20%) 1 0	30, 107, 141, 158	0
1	G	162/198 (81%)	0.16	8 (4%) 29 26	41, 71, 110, 128	0
1	I	169/198 (85%)	-0.13	3 (1%) 68 67	31, 49, 89, 115	0
1	K	136/198 (68%)	0.49	12 (8%) 10 7	65, 108, 153, 181	0
2	B	45/54 (83%)	0.12	0 100 100	46, 53, 77, 89	0
2	D	46/54 (85%)	0.11	0 100 100	39, 65, 92, 97	0
2	F	40/54 (74%)	1.63	15 (37%) 0 0	115, 138, 166, 172	0
2	H	45/54 (83%)	-0.06	0 100 100	54, 63, 77, 86	0
2	J	43/54 (79%)	0.42	6 (13%) 2 2	59, 80, 107, 120	0
2	L	14/54 (25%)	2.17	7 (50%) 0 0	111, 132, 161, 165	0
All	All	1171/1512 (77%)	0.21	80 (6%) 17 13	20, 65, 136, 181	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	81	TYR	9.3
1	K	26	TRP	7.2
1	E	85	SER	5.8
1	E	26	TRP	5.3
2	F	88	LEU	5.3
2	F	91	ASN	5.2
2	F	83	ILE	5.1
2	L	85	LEU	4.9
2	F	90	GLY	4.7
1	E	23	ASN	4.6
1	E	144	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	79	GLU	4.1
2	L	86	HIS	4.0
1	C	205	ALA	3.9
2	F	96	ILE	3.9
1	K	200	THR	3.8
1	I	11	ASP	3.8
2	F	104	THR	3.8
1	K	127	ASN	3.7
1	E	80	LEU	3.7
1	A	87	ALA	3.5
1	E	79	GLU	3.4
1	G	106	LEU	3.4
2	F	89	LEU	3.4
1	E	82	GLU	3.4
2	L	79	GLU	3.4
1	E	83	SER	3.4
2	F	111	TYR	3.4
1	G	105	ALA	3.3
1	E	74	SER	3.3
1	E	86	LEU	3.3
2	F	79	GLU	3.2
2	F	87	LYS	3.1
2	L	81	LEU	3.1
2	L	84	ARG	3.1
1	G	38	GLN	2.7
1	K	155	VAL	2.7
1	K	81	TYR	2.7
1	K	77	LEU	2.7
1	I	68	GLN	2.7
2	F	77	GLN	2.7
2	L	80	ASP	2.7
1	K	123	SER	2.6
1	E	110	ASP	2.6
1	E	130	GLU	2.6
1	E	173	PHE	2.6
1	I	37	SER	2.6
1	G	121	CYS	2.6
1	K	84	LEU	2.5
1	E	161	LEU	2.5
2	J	112	TRP	2.5
1	E	71	LEU	2.5
2	J	115	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	111	LEU	2.5
1	K	47	GLY	2.5
1	G	191	ASP	2.4
2	J	93	TRP	2.4
1	G	23	ASN	2.4
2	F	78	GLU	2.4
2	F	97	ALA	2.4
2	F	84	ARG	2.4
1	E	163	LYS	2.4
1	A	54	LYS	2.3
1	E	162	ALA	2.3
2	L	83	ILE	2.3
1	E	189	LYS	2.2
2	J	113	ASN	2.2
1	E	136	ALA	2.2
2	F	110	ASN	2.2
1	K	45	GLY	2.1
1	K	157	THR	2.1
2	J	110	ASN	2.1
1	G	114	THR	2.1
1	E	31	PHE	2.1
1	E	147	ASN	2.1
1	E	191	ASP	2.1
1	E	27	SER	2.1
2	J	107	GLN	2.0
1	G	19	VAL	2.0
1	E	33	SER	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 monosaccharides 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.