



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 7FDL / pdb_00007fdl
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	:	4-5-2 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

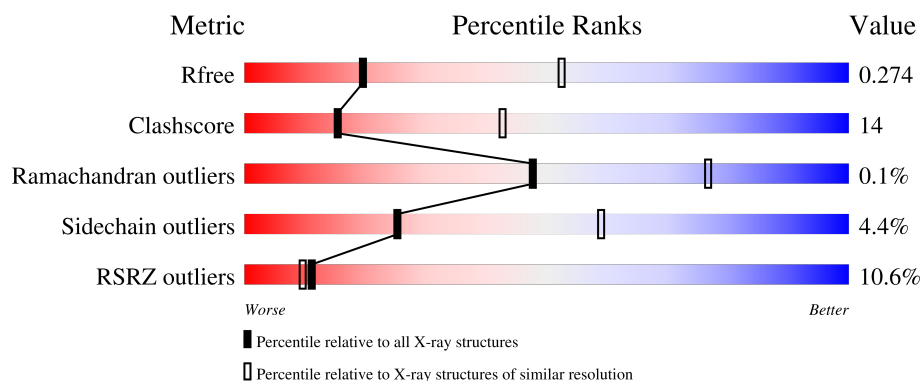
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	2% 61% 27% 12%
1	C	198	% 65% 21% 14%
1	E	198	23% 48% 13% 37%
1	G	198	4% 59% 22% 18%
1	I	198	2% 61% 23% 15%

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Mol	Chain	Length	Quality of chain
1	K	198	18%49%18%•31%
2	B	54	2%56%24%•17%
2	D	54	2%63%20%•15%
2	F	54	33%67%6%•26%
2	H	54	2%48%33%•17%
2	J	54	4%46%31%•20%
2	L	54	9%22%•74%

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			

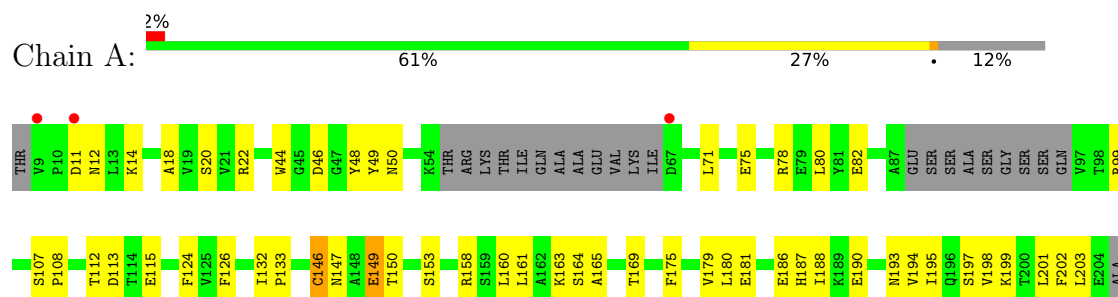
- Molecule 2 is a protein called Transcription factor WER.

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			

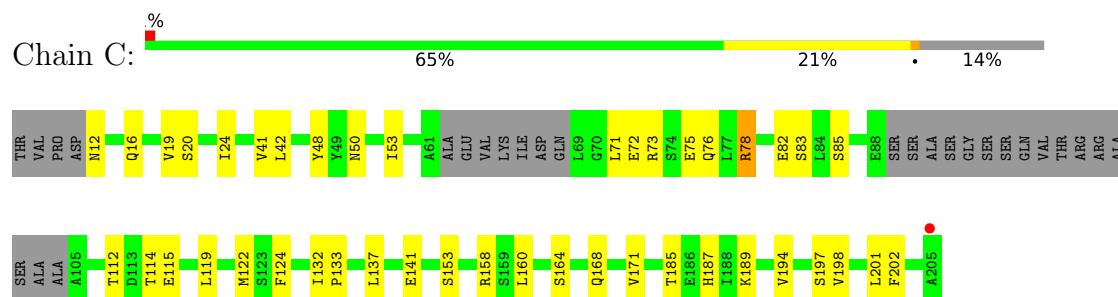
3 Residue-property plots [i](#)

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.

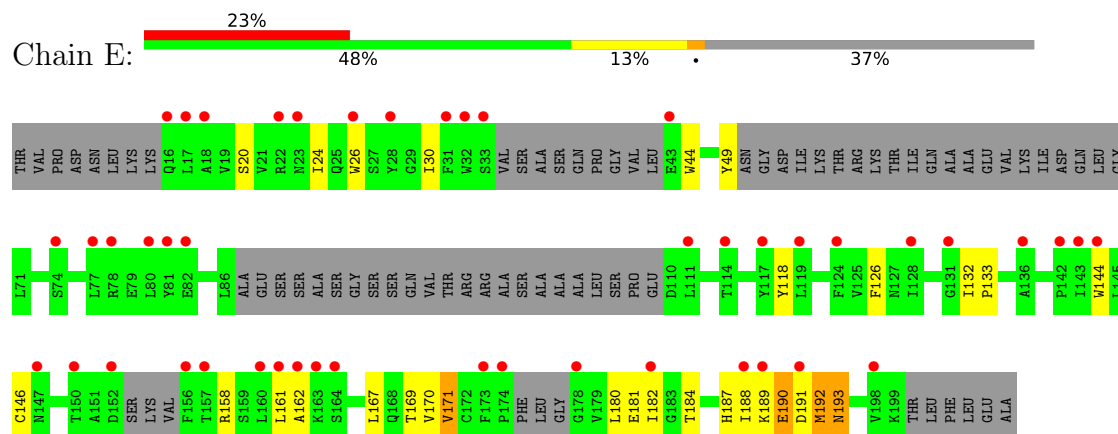
• Molecule 1: Transcription factor EGL1



• Molecule 1: Transcription factor EGL1

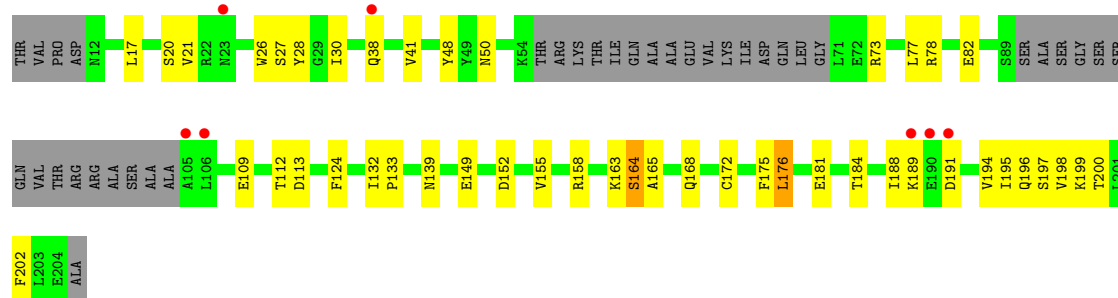


• Molecule 1: Transcription factor EGL1

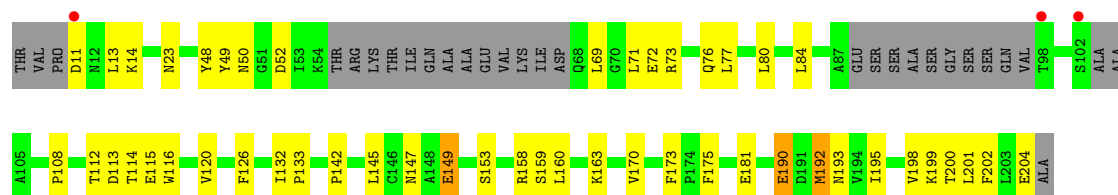


• Molecule 1: Transcription factor EGL1

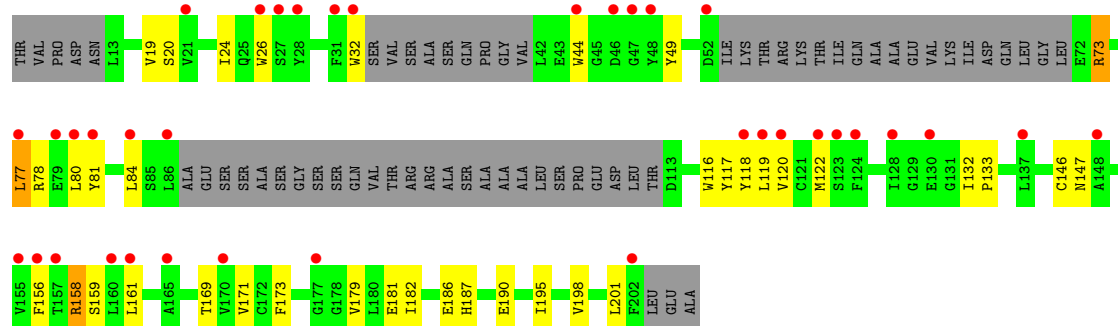




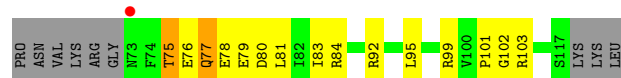
- Molecule 1: Transcription factor EGL1



- Molecule 1: Transcription factor EGL1



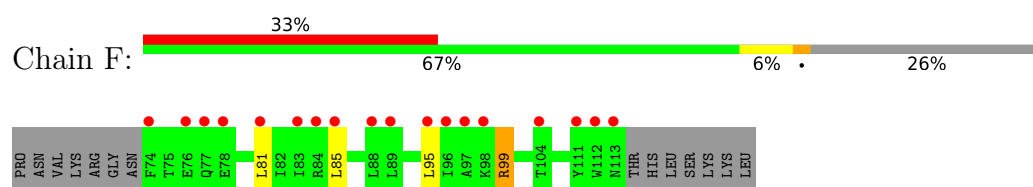
- Molecule 2: Transcription factor WER



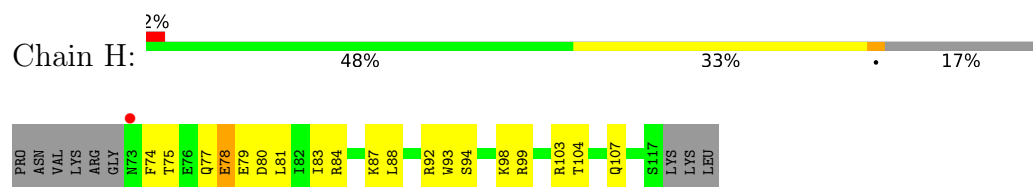
- Molecule 2: Transcription factor WER



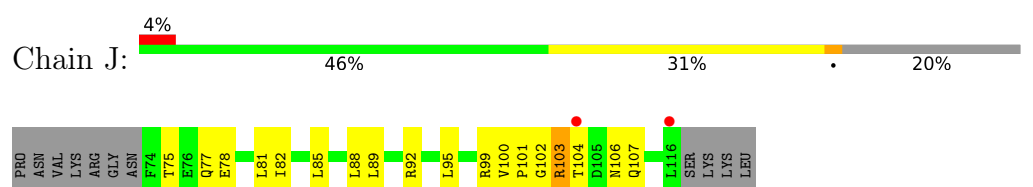
- Molecule 2: Transcription factor WER



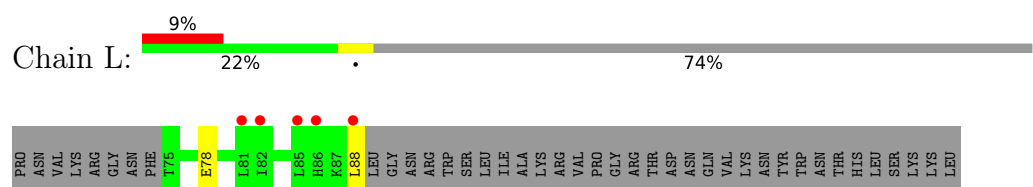
• Molecule 2: Transcription factor WER



• 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) 84.8 (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 (4.19%)	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)	0.29 , 48.6	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	0.87	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

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	0.59	1/1361 (0.1%)	0.73	5/1850 (0.3%)
1	C	0.54	0/1345	0.60	0/1825
1	E	0.53	1/944 (0.1%)	0.68	1/1284 (0.1%)
1	G	0.38	0/1222	0.64	1/1667 (0.1%)
1	I	0.37	0/1321	0.60	0/1794
1	K	0.43	0/955	0.77	5/1306 (0.4%)
2	B	0.66	0/384	0.71	1/519 (0.2%)
2	D	0.32	0/393	0.50	0/531
2	F	0.23	0/276	0.47	0/380
2	H	0.30	0/387	0.64	0/523
2	J	0.46	0/358	0.97	4/486 (0.8%)
2	L	0.34	0/95	0.56	0/128
All	All	0.47	2/9041 (0.0%)	0.67	17/12293 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	SER	CA-C	7.01	1.59	1.52
1	E	190	GLU	CA-C	-5.12	1.46	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	78	ARG	CA-C-N	9.06	132.22	120.44
1	K	78	ARG	C-N-CA	9.06	132.22	120.44
1	K	73	ARG	N-CA-C	8.74	120.81	111.28
1	E	193	ASN	N-CA-C	8.60	120.66	111.28
1	A	107	SER	O-C-N	7.79	127.41	121.88
1	K	78	ARG	N-CA-C	6.45	118.39	111.36
1	K	77	LEU	N-CA-C	5.81	117.29	111.07
2	J	104	THR	CA-C-N	-5.80	110.27	121.58
2	J	104	THR	C-N-CA	-5.80	110.27	121.58
1	A	11	ASP	N-CA-C	5.75	117.80	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	106	ASN	N-CA-C	5.60	120.24	112.45
1	A	12	ASN	N-CA-C	-5.59	100.66	108.54
2	J	104	THR	O-C-N	-5.36	115.04	122.76
1	A	12	ASN	CA-C-N	5.11	127.55	120.29
1	A	12	ASN	C-N-CA	5.11	127.55	120.29
1	G	189	LYS	N-CA-C	5.09	117.20	108.90
2	B	75	THR	N-CA-C	-5.01	103.44	110.50

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	1334	0	1291	41	0
1	C	1319	0	1283	24	0
1	E	925	0	807	33	0
1	G	1196	0	1105	37	0
1	I	1296	0	1230	37	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	16	0
2	J	351	0	345	17	0
2	L	96	0	75	2	0
All	All	8866	0	8277	231	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 14.

All (231) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ2	1:G:168:GLN:CB	1.91	0.83
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:E:192:MET:HE2	1:E:192:MET:HA	1.66	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
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:189:LYS:HZ1	1:G:168:GLN:CB	2.07	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: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:E:192:MET:HA	1:E:192:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:93:TRP:H	2:H:93:TRP:CD1	2.19	0.60
2:B:102:GLY:C	2:B:103:ARG:HD3	2.27	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:187:HIS:C	1:A:188:ILE:HD13	2.28	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
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:E:188:ILE:HD12	1:E:188:ILE:C	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:LEU:C	2:L:88:LEU:HD12	2.36	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:E:191:ASP:C	1:E:193:ASN:N	2.67	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: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
2:J:102:GLY:C	2:J:103:ARG:HD3	2.39	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:A:199:LYS:NZ	1:C:141:GLU:OE1	2.37	0.47
1:E:190:GLU:O	1:E:190:GLU:HG2	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
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:K:119:LEU:C	1:K:119:LEU:HD23	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:146:CYS:O	1:K:147:ASN:C	2.59	0.44
1:E:192:MET:HB2	1:E:192:MET:HE3	1.61	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:191:ASP:C	1:E:193:ASN:H	2.25	0.44
1:C:119:LEU:HA	1:C:122:MET:HE2	1.99	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: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
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:192:MET:HE2	1:I:195:ILE:HD12	2.00	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:17:LEU:O	1:G:21:VAL:HG22	2.20	0.40
1:A:146:CYS:O	1:A:147:ASN:C	2.64	0.40
2:H:87:LYS:C	2:H:88:LEU:HD23	2.46	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	51
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%)	48	77

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%)	22	53
1	C	142/167 (85%)	135 (95%)	7 (5%)	22	54
1	E	87/167 (52%)	84 (97%)	3 (3%)	32	66
1	G	119/167 (71%)	116 (98%)	3 (2%)	42	74
1	I	138/167 (83%)	132 (96%)	6 (4%)	26	60
1	K	81/167 (48%)	77 (95%)	4 (5%)	22	54
2	B	40/50 (80%)	38 (95%)	2 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	41/50 (82%)	39 (95%)	2 (5%)	22	54
2	F	19/50 (38%)	18 (95%)	1 (5%)	20	52
2	H	41/50 (82%)	40 (98%)	1 (2%)	43	75
2	J	36/50 (72%)	34 (94%)	2 (6%)	19	50
2	L	7/50 (14%)	6 (86%)	1 (14%)	3	11
All	All	891/1302 (68%)	852 (96%)	39 (4%)	25	59

All (39) 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	78	ARG
1	C	83	SER
1	C	114	THR
1	C	164	SER
1	C	171	VAL
1	C	189	LYS
2	D	99	ARG
2	D	104	THR
1	E	144	TRP
1	E	171	VAL
1	E	192	MET
2	F	99	ARG
1	G	20	SER
1	G	164	SER
1	G	176	LEU
2	H	78	GLU
1	I	52	ASP
1	I	149	GLU
1	I	159	SER
1	I	190	GLU

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Mol	Chain	Res	Type
1	I	192	MET
1	I	193	ASN
2	J	103	ARG
2	J	107	GLN
1	K	73	ARG
1	K	77	LEU
1	K	80	LEU
1	K	158	ARG
2	L	78	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	187	HIS
2	B	113	ASN
1	C	50	ASN
1	C	76	GLN
1	C	193	ASN
1	C	196	GLN
2	D	107	GLN
2	D	115	HIS
1	E	139	ASN
1	E	187	HIS
2	H	86	HIS
2	H	91	ASN
2	H	107	GLN
1	I	12	ASN
1	I	147	ASN
1	K	187	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	175/198 (88%)	-0.04	3 (1%) 69 61	32, 46, 76, 92	0
1	C	171/198 (86%)	-0.28	1 (0%) 85 81	20, 33, 71, 101	0
1	E	125/198 (63%)	1.71	46 (36%) 1 0	30, 107, 141, 158	0
1	G	162/198 (81%)	0.39	7 (4%) 40 31	41, 71, 110, 128	0
1	I	169/198 (85%)	0.09	3 (1%) 67 59	31, 49, 89, 115	0
1	K	136/198 (68%)	1.54	36 (26%) 1 1	65, 108, 153, 181	0
2	B	45/54 (83%)	0.24	1 (2%) 62 53	46, 53, 77, 89	0
2	D	46/54 (85%)	0.17	1 (2%) 62 53	39, 65, 92, 97	0
2	F	40/54 (74%)	1.99	18 (45%) 0 0	115, 138, 166, 172	0
2	H	45/54 (83%)	0.15	1 (2%) 62 53	54, 63, 77, 86	0
2	J	43/54 (79%)	0.56	2 (4%) 36 28	59, 80, 107, 120	0
2	L	14/54 (25%)	1.53	5 (35%) 1 0	111, 132, 161, 165	0
All	All	1171/1512 (77%)	0.51	124 (10%) 11 9	20, 65, 136, 181	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	81	TYR	6.7
1	K	26	TRP	6.4
1	K	77	LEU	5.4
1	E	152	ASP	5.2
2	F	77	GLN	4.8
1	K	170	VAL	4.8
1	E	33	SER	4.8
1	E	144	TRP	4.3
1	E	163	LYS	4.3
1	K	80	LEU	4.2
1	K	86	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	161	LEU	4.1
2	B	73	ASN	4.0
1	K	160	LEU	4.0
1	E	191	ASP	4.0
1	K	47	GLY	4.0
1	E	43	GLU	3.7
1	K	46	ASP	3.7
2	L	88	LEU	3.7
1	E	26	TRP	3.7
2	F	78	GLU	3.6
1	I	11	ASP	3.5
1	K	48	TYR	3.4
1	K	157	THR	3.4
1	E	173	PHE	3.3
1	I	98	THR	3.3
1	C	205	ALA	3.3
2	J	116	LEU	3.3
2	J	104	THR	3.3
2	F	96	ILE	3.2
2	F	83	ILE	3.2
1	E	119	LEU	3.2
1	E	160	LEU	3.2
1	E	161	LEU	3.2
1	E	17	LEU	3.1
1	E	77	LEU	3.1
2	F	95	LEU	3.1
1	A	67	ASP	3.1
2	L	85	LEU	3.1
1	E	74	SER	3.1
1	E	16	GLN	3.1
1	E	157	THR	3.1
1	K	123	SER	3.0
1	E	189	LYS	3.0
2	H	73	ASN	3.0
1	K	84	LEU	3.0
1	K	118	TYR	2.9
2	F	88	LEU	2.9
1	E	142	PRO	2.9
2	F	113	ASN	2.9
1	K	148	ALA	2.9
2	F	97	ALA	2.9
2	L	86	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	81	LEU	2.9
1	G	191	ASP	2.9
1	K	137	LEU	2.9
1	A	11	ASP	2.9
1	K	28	TYR	2.8
2	F	111	TYR	2.8
2	F	81	LEU	2.8
1	K	27	SER	2.8
1	E	178	GLY	2.8
1	K	32	TRP	2.8
1	E	156	PHE	2.8
1	E	22	ARG	2.7
2	F	84	ARG	2.7
1	K	124	PHE	2.7
1	E	162	ALA	2.7
1	K	165	ALA	2.7
1	E	147	ASN	2.7
2	F	85	LEU	2.7
1	E	150	THR	2.7
2	L	82	ILE	2.6
1	E	136	ALA	2.6
1	E	111	LEU	2.6
2	D	117	SER	2.6
2	F	104	THR	2.6
1	K	52	ASP	2.6
1	K	81	TYR	2.6
1	K	156	PHE	2.6
1	E	78	ARG	2.5
1	E	80	LEU	2.5
1	E	131	GLY	2.5
1	G	190	GLU	2.5
1	E	188	ILE	2.5
1	K	31	PHE	2.5
1	E	23	ASN	2.5
1	K	177	GLY	2.4
1	K	44	TRP	2.4
1	K	122	MET	2.4
1	E	32	TRP	2.4
1	K	119	LEU	2.4
2	F	89	LEU	2.4
2	F	74	PHE	2.4
1	E	114	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	82	GLU	2.4
1	K	130	GLU	2.4
1	E	182	ILE	2.4
1	K	21	VAL	2.3
1	K	120	VAL	2.3
1	E	31	PHE	2.3
1	A	9	VAL	2.3
1	G	189	LYS	2.3
1	I	102	SER	2.3
1	E	117	TYR	2.3
1	E	124	PHE	2.2
2	F	112	TRP	2.2
1	E	174	PRO	2.2
1	E	198	VAL	2.2
1	K	155	VAL	2.2
1	E	128	ILE	2.2
1	G	23	ASN	2.2
1	E	143	ILE	2.1
2	F	76	GLU	2.1
2	F	98	LYS	2.1
1	K	128	ILE	2.1
1	G	106	LEU	2.1
1	G	105	ALA	2.1
1	K	202	PHE	2.0
1	E	18	ALA	2.0
1	K	79	GLU	2.0
1	E	28	TYR	2.0
1	E	164	SER	2.0
1	G	38	GLN	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.