



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 PM UTC

PDB ID : 2AUK / pdb_00002auk
Title : Structure of E. coli RNA polymerase beta' G/G' insert
Authors : Chlenov, M.; Masuda, S.; Murakami, K.S.; Nikiforov, V.; Darst, S.A.; Mustaev, A.
Deposited on : 2005-08-28
Resolution : 2.30 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

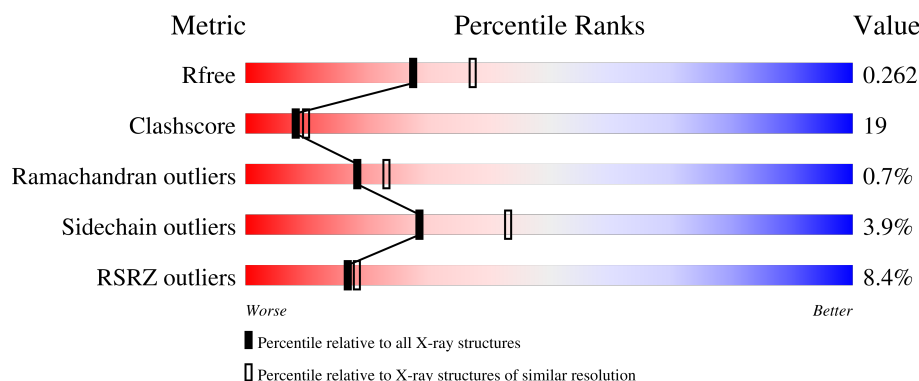
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	190	6% 65% 31% ..
1	B	190	3% 66% 26% 5%
1	C	190	4% 74% 20% ..
1	D	190	15% 62% 31% ..
1	E	190	14% 61% 35% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7306 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 DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1401	872	240	285	4			
1	B	181	Total	C	N	O	S	0	0	0
			1354	845	232	274	3			
1	C	183	Total	C	N	O	S	0	0	0
			1364	851	234	276	3			
1	D	183	Total	C	N	O	S	0	0	0
			1351	842	233	273	3			
1	E	188	Total	C	N	O	S	0	0	0
			1379	861	235	279	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P0A8T7
A	2	SER	-	cloning artifact	UNP P0A8T7
A	3	HIS	-	cloning artifact	UNP P0A8T7
A	4	MET	-	cloning artifact	UNP P0A8T7
B	1	GLY	-	cloning artifact	UNP P0A8T7
B	2	SER	-	cloning artifact	UNP P0A8T7
B	3	HIS	-	cloning artifact	UNP P0A8T7
B	4	MET	-	cloning artifact	UNP P0A8T7
C	1	GLY	-	cloning artifact	UNP P0A8T7
C	2	SER	-	cloning artifact	UNP P0A8T7
C	3	HIS	-	cloning artifact	UNP P0A8T7
C	4	MET	-	cloning artifact	UNP P0A8T7
D	1	GLY	-	cloning artifact	UNP P0A8T7
D	2	SER	-	cloning artifact	UNP P0A8T7
D	3	HIS	-	cloning artifact	UNP P0A8T7
D	4	MET	-	cloning artifact	UNP P0A8T7
E	1	GLY	-	cloning artifact	UNP P0A8T7
E	2	SER	-	cloning artifact	UNP P0A8T7
E	3	HIS	-	cloning artifact	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	4	MET	-	cloning artifact	UNP P0A8T7

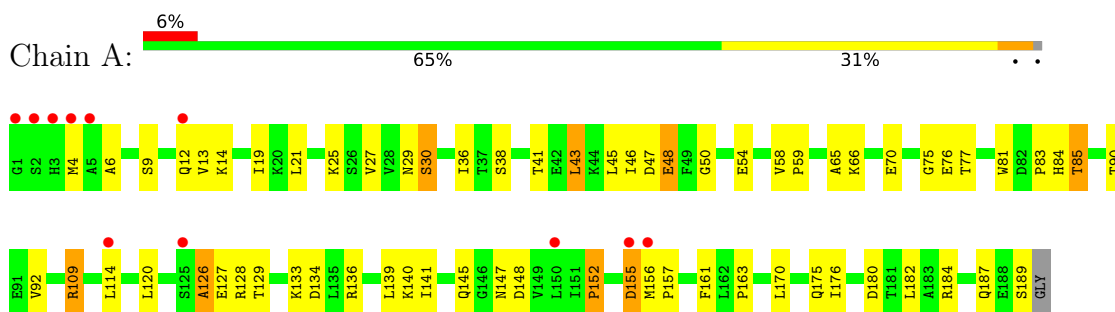
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total 97	O 97	0	0
2	B	111	Total 111	O 111	0	0
2	C	91	Total 91	O 91	0	0
2	D	87	Total 87	O 87	0	0
2	E	71	Total 71	O 71	0	0

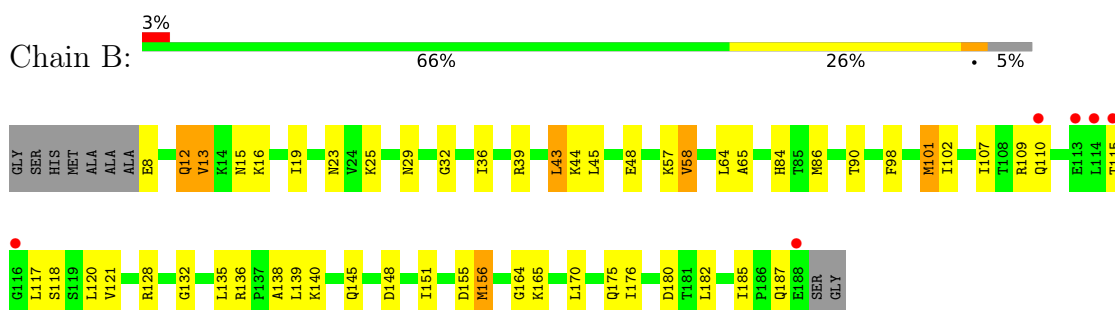
3 Residue-property plots

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.

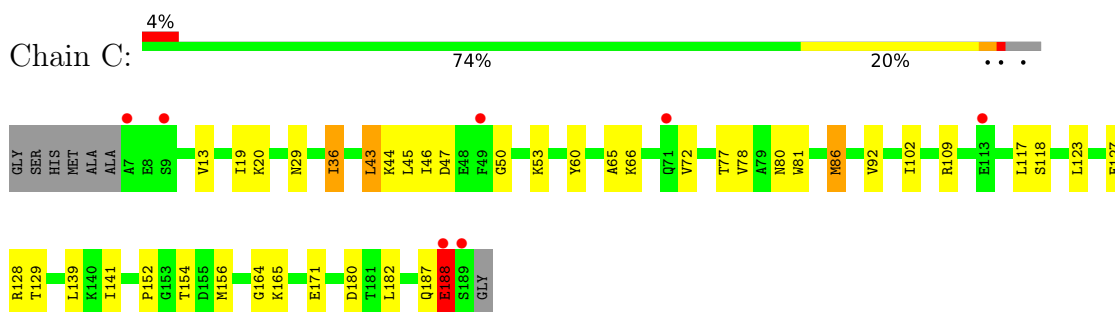
- Molecule 1: DNA-directed RNA polymerase beta' chain



- Molecule 1: DNA-directed RNA polymerase beta' chain

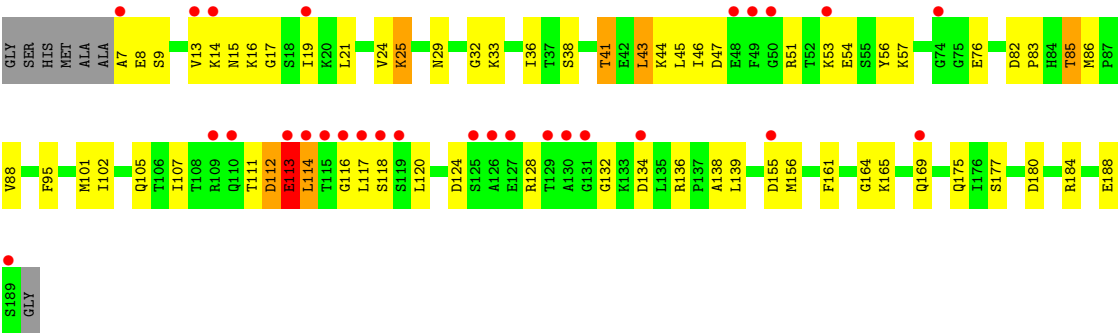


- Molecule 1: DNA-directed RNA polymerase beta' chain

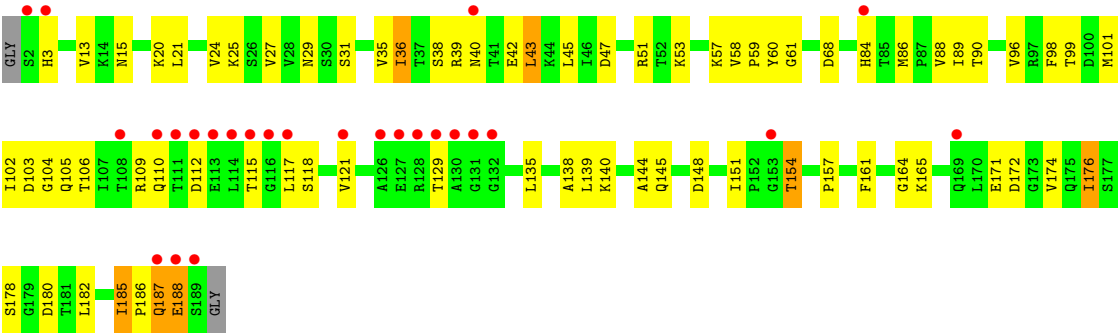


- Molecule 1: DNA-directed RNA polymerase beta' chain





● Molecule 1: DNA-directed RNA polymerase beta' chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.03Å 95.13Å 86.07Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30 35.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.30) 91.7 (35.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.264 0.220 , 0.262	Depositor DCC
R_{free} test set	3528 reflections (8.12%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7306	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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	0.45	0/1418	0.97	2/1920 (0.1%)
1	B	0.50	1/1371 (0.1%)	1.00	8/1857 (0.4%)
1	C	0.49	0/1381	0.99	5/1871 (0.3%)
1	D	0.53	1/1368 (0.1%)	0.99	4/1855 (0.2%)
1	E	0.45	0/1396	0.95	6/1893 (0.3%)
All	All	0.48	2/6934 (0.0%)	0.98	25/9396 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	GLU	CA-CB	8.09	1.67	1.53
1	B	101	MET	SD-CE	-5.06	1.67	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	THR	N-CA-C	-9.38	96.99	110.59
1	C	188	GLU	N-CA-C	9.35	130.71	110.80
1	D	112	ASP	N-CA-C	-8.14	103.44	112.72
1	B	151	ILE	N-CA-C	-7.36	101.73	108.95
1	A	114	LEU	N-CA-C	6.90	118.69	111.03
1	D	88	VAL	N-CA-C	-6.69	98.22	107.99
1	B	16	LYS	N-CA-C	-6.44	100.03	110.20
1	E	185	ILE	CA-C-N	6.25	126.22	119.78
1	E	185	ILE	C-N-CA	6.25	126.22	119.78
1	D	117	LEU	N-CA-C	-6.12	104.72	111.82
1	B	185	ILE	CA-C-N	6.05	126.02	120.21
1	B	185	ILE	C-N-CA	6.05	126.02	120.21
1	B	58	VAL	CA-C-N	5.96	125.92	119.78
1	B	58	VAL	C-N-CA	5.96	125.92	119.78
1	B	25	LYS	N-CA-C	-5.92	98.76	108.76
1	C	86	MET	CA-C-N	-5.62	114.78	120.85
1	C	86	MET	C-N-CA	-5.62	114.78	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	THR	N-CA-C	-5.59	103.00	110.55
1	B	155	ASP	N-CA-C	-5.47	105.92	112.59
1	A	155	ASP	N-CA-C	-5.39	106.01	112.59
1	C	128	ARG	N-CA-C	5.35	117.77	110.55
1	D	25	LYS	N-CA-C	-5.25	100.13	109.06
1	E	24	VAL	N-CA-C	5.14	115.88	108.48
1	E	31	SER	N-CA-C	-5.13	106.61	112.92
1	E	88	VAL	N-CA-C	-5.01	100.68	107.99

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	1401	0	1415	59	0
1	B	1354	0	1372	57	0
1	C	1364	0	1379	38	0
1	D	1351	0	1350	67	0
1	E	1379	0	1384	66	0
2	A	97	0	0	7	0
2	B	111	0	0	7	0
2	C	91	0	0	4	0
2	D	87	0	0	9	0
2	E	71	0	0	7	0
All	All	7306	0	6900	265	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 19.

All (265) 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:65:ALA:HB2	1:D:156:MET:HE2	1.31	1.10
1:A:85:THR:HG21	1:A:184:ARG:HD3	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HE3	1:C:77:THR:HG22	1.42	0.99
1:B:107:ILE:HD12	1:B:120:LEU:HD22	1.50	0.93
1:E:101:MET:HE1	1:E:139:LEU:HD23	1.52	0.91
1:D:21:LEU:HB3	1:D:24:VAL:HG11	1.54	0.88
1:A:4:MET:HE3	1:A:6:ALA:HB3	1.54	0.88
1:D:45:LEU:HB2	1:D:54:GLU:HB2	1.56	0.87
1:B:101:MET:HE1	1:B:139:LEU:HD23	1.56	0.84
1:E:3:HIS:HA	2:E:192:HOH:O	1.78	0.82
1:B:13:VAL:HG21	1:B:45:LEU:HD13	1.64	0.80
1:D:114:LEU:N	1:D:114:LEU:HD23	1.99	0.78
1:C:47:ASP:OD2	1:C:53:LYS:HE2	1.82	0.78
1:B:101:MET:HE2	1:B:138:ALA:O	1.83	0.78
1:E:187:GLN:HG2	1:E:188:GLU:H	1.49	0.77
1:D:9:SER:HB3	1:D:83:PRO:HG3	1.65	0.77
1:B:140:LYS:HZ1	1:B:148:ASP:CG	1.92	0.76
1:D:101:MET:HE1	1:D:139:LEU:HD23	1.66	0.76
1:C:154:THR:HG22	1:C:156:MET:HB2	1.66	0.75
1:D:47:ASP:OD2	1:D:53:LYS:HE3	1.87	0.74
1:D:114:LEU:HD23	1:D:114:LEU:H	1.53	0.74
1:B:57:LYS:HD3	1:C:171:GLU:HG2	1.67	0.74
1:E:13:VAL:HG21	1:E:45:LEU:HD13	1.69	0.74
1:A:77:THR:OG1	1:D:155:ASP:HB3	1.88	0.73
1:D:85:THR:HG21	1:D:184:ARG:HD3	1.70	0.73
1:B:29:ASN:HB2	1:B:180:ASP:OD1	1.88	0.73
1:C:86:MET:HE2	2:C:192:HOH:O	1.88	0.72
1:E:21:LEU:HD21	1:E:43:LEU:HD22	1.71	0.72
1:A:84:HIS:O	1:A:187:GLN:HG3	1.90	0.71
1:B:13:VAL:HG22	1:B:45:LEU:HD22	1.72	0.71
1:B:136:ARG:HH11	1:B:136:ARG:HG2	1.55	0.71
1:E:25:LYS:HB2	1:E:38:SER:HB3	1.72	0.70
1:D:111:THR:HG23	1:D:116:GLY:O	1.92	0.70
1:D:111:THR:HG22	1:D:113:GLU:H	1.57	0.69
1:E:117:LEU:HD23	2:E:238:HOH:O	1.91	0.69
1:A:136:ARG:CZ	2:A:229:HOH:O	2.40	0.69
1:D:43:LEU:HD12	1:D:44:LYS:N	2.07	0.69
1:D:9:SER:CB	1:D:83:PRO:HG3	2.24	0.68
1:E:29:ASN:HB2	1:E:180:ASP:OD1	1.94	0.67
1:E:98:PHE:HA	1:E:101:MET:HE3	1.75	0.67
1:D:21:LEU:HB3	1:D:24:VAL:CG1	2.24	0.66
1:A:85:THR:HG22	2:A:208:HOH:O	1.95	0.66
1:E:151:ILE:O	1:E:154:THR:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:MET:HB2	1:C:187:GLN:NE2	2.09	0.65
1:E:101:MET:HE2	1:E:138:ALA:O	1.96	0.65
1:C:29:ASN:HB2	1:C:180:ASP:OD1	1.96	0.65
1:A:21:LEU:HD21	1:A:43:LEU:HD22	1.79	0.65
1:C:164:GLY:O	1:C:165:LYS:HB2	1.97	0.64
1:D:101:MET:HE1	1:D:139:LEU:CD2	2.26	0.64
1:C:46:ILE:CG2	1:C:50:GLY:HA2	2.27	0.64
1:A:155:ASP:O	1:A:157:PRO:HD3	1.98	0.64
1:D:169:GLN:HA	2:D:221:HOH:O	1.97	0.64
1:E:47:ASP:OD2	1:E:51:ARG:HB2	1.98	0.64
1:B:140:LYS:NZ	1:B:148:ASP:CG	2.56	0.63
1:D:14:LYS:HG3	2:D:248:HOH:O	1.98	0.63
1:B:98:PHE:HA	1:B:101:MET:CE	2.29	0.63
1:E:13:VAL:HG22	1:E:45:LEU:HD22	1.81	0.63
1:B:57:LYS:HD3	1:C:171:GLU:CG	2.29	0.63
1:E:15:ASN:HB2	1:E:45:LEU:HD21	1.81	0.62
1:E:27:VAL:HG21	1:E:178:SER:HB2	1.81	0.62
1:B:15:ASN:HB2	1:B:45:LEU:HD21	1.81	0.62
1:B:98:PHE:HA	1:B:101:MET:HE3	1.81	0.62
1:A:136:ARG:NH1	2:A:229:HOH:O	2.32	0.62
1:C:66:LYS:HD2	1:C:72:VAL:HG12	1.82	0.62
1:D:111:THR:HA	1:D:116:GLY:O	2.00	0.62
1:E:112:ASP:HB2	1:E:115:THR:HB	1.81	0.62
1:D:177:SER:HB2	1:E:86:MET:HE1	1.82	0.62
1:A:13:VAL:HG21	1:A:45:LEU:HD13	1.81	0.62
1:C:13:VAL:HG13	1:C:45:LEU:HD22	1.81	0.61
1:A:19:ILE:HD12	1:A:43:LEU:HD11	1.82	0.61
1:A:129:THR:O	1:A:133:LYS:HG2	1.99	0.61
1:A:152:PRO:HB2	2:A:217:HOH:O	2.01	0.61
1:D:169:GLN:HB2	2:D:206:HOH:O	2.00	0.61
1:D:17:GLY:HA3	1:D:46:ILE:O	2.01	0.60
1:B:39:ARG:HD3	2:B:264:HOH:O	2.00	0.60
1:D:19:ILE:HG23	1:D:43:LEU:HD11	1.82	0.60
1:B:43:LEU:HD12	1:B:43:LEU:C	2.27	0.60
1:E:101:MET:HE1	1:E:139:LEU:CD2	2.29	0.60
1:A:170:LEU:HD13	1:A:176:ILE:HG22	1.85	0.59
1:D:36:ILE:HG21	1:D:41:THR:HG21	1.85	0.59
1:D:112:ASP:O	1:D:114:LEU:N	2.30	0.59
1:B:43:LEU:HD12	1:B:44:LYS:N	2.18	0.58
1:B:136:ARG:HG2	1:B:136:ARG:NH1	2.16	0.58
1:E:98:PHE:HA	1:E:101:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG23	1:A:43:LEU:HD13	1.85	0.58
1:B:132:GLY:HA2	1:B:135:LEU:HD12	1.86	0.57
1:E:21:LEU:CD2	1:E:43:LEU:HD22	2.33	0.57
1:B:98:PHE:CA	1:B:101:MET:HE3	2.35	0.56
1:C:19:ILE:HG23	1:C:43:LEU:CD1	2.34	0.56
1:B:101:MET:HE1	1:B:139:LEU:CD2	2.32	0.56
1:D:128:ARG:HB3	1:D:132:GLY:HA3	1.87	0.56
1:E:115:THR:HA	2:E:232:HOH:O	2.05	0.55
1:A:84:HIS:HA	1:A:187:GLN:CD	2.30	0.55
1:A:36:ILE:HD12	1:A:58:VAL:HG11	1.89	0.55
1:E:47:ASP:OD2	1:E:53:LYS:HE2	2.07	0.55
1:E:98:PHE:CA	1:E:101:MET:HE3	2.36	0.55
1:C:92:VAL:HG23	1:C:141:ILE:HG21	1.88	0.55
1:D:41:THR:HG23	2:D:191:HOH:O	2.05	0.55
1:E:35:VAL:HG11	1:E:89:ILE:HD13	1.89	0.55
1:A:48:GLU:CD	1:A:48:GLU:H	2.14	0.55
1:C:154:THR:CG2	1:C:156:MET:HB2	2.35	0.55
1:E:140:LYS:HE3	2:E:225:HOH:O	2.06	0.55
1:B:156:MET:CE	1:C:65:ALA:HB2	2.37	0.54
1:D:13:VAL:HG23	1:D:76:GLU:O	2.08	0.54
1:B:84:HIS:O	1:B:187:GLN:HG3	2.08	0.54
1:C:43:LEU:HD12	1:C:44:LYS:N	2.22	0.54
1:A:29:ASN:HB2	1:A:180:ASP:OD1	2.09	0.53
1:B:13:VAL:CG2	1:B:45:LEU:HD13	2.34	0.53
1:D:15:ASN:ND2	1:D:53:LYS:HD3	2.23	0.53
1:E:86:MET:HB3	2:E:204:HOH:O	2.08	0.53
1:E:144:ALA:HB3	1:E:145:GLN:NE2	2.23	0.53
1:A:85:THR:HG21	1:A:184:ARG:HB3	1.91	0.53
1:C:156:MET:HG2	2:C:257:HOH:O	2.08	0.53
1:C:43:LEU:HD12	1:C:43:LEU:C	2.34	0.53
1:D:107:ILE:HD12	1:D:120:LEU:HD22	1.90	0.53
1:D:118:SER:CB	1:E:42:GLU:OE2	2.57	0.52
1:A:65:ALA:CB	1:D:156:MET:HE2	2.20	0.52
1:B:115:THR:HG22	1:B:117:LEU:HG	1.90	0.52
1:A:47:ASP:HB2	1:A:48:GLU:OE2	2.10	0.52
1:B:15:ASN:HB2	1:B:45:LEU:CD2	2.38	0.52
1:B:156:MET:CE	1:C:77:THR:HG22	2.26	0.52
1:E:106:THR:HG23	1:E:135:LEU:HD12	1.92	0.52
1:D:102:ILE:N	1:D:102:ILE:HD12	2.25	0.52
1:A:85:THR:CG2	1:A:184:ARG:HB3	2.39	0.51
1:D:7:ALA:C	1:D:9:SER:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:176:ILE:HD11	1.92	0.51
1:A:13:VAL:CG2	1:A:45:LEU:HD22	2.41	0.51
1:A:136:ARG:NH1	2:A:283:HOH:O	2.43	0.51
1:A:156:MET:SD	1:B:65:ALA:HB2	2.50	0.51
1:A:134:ASP:C	2:A:229:HOH:O	2.52	0.51
1:B:170:LEU:HD12	1:B:170:LEU:C	2.36	0.51
1:C:19:ILE:HG23	1:C:43:LEU:HD11	1.93	0.51
1:D:32:GLY:HA2	1:E:161:PHE:O	2.11	0.51
1:D:43:LEU:HD12	1:D:43:LEU:C	2.35	0.51
1:B:110:GLN:NE2	1:B:121:VAL:HG21	2.26	0.51
1:C:102:ILE:HD12	1:C:102:ILE:N	2.25	0.51
1:A:139:LEU:HD12	1:A:182:LEU:HB3	1.93	0.51
1:D:47:ASP:OD2	1:D:51:ARG:HB2	2.10	0.51
1:D:25:LYS:HB2	1:D:38:SER:HB3	1.93	0.50
1:A:13:VAL:HG22	1:A:45:LEU:HD22	1.94	0.50
1:E:84:HIS:CD2	1:E:187:GLN:HE22	2.29	0.50
1:B:102:ILE:N	1:B:102:ILE:HD12	2.26	0.50
1:D:24:VAL:HG12	1:D:41:THR:HB	1.94	0.50
1:D:118:SER:CB	1:E:57:LYS:NZ	2.75	0.50
1:B:36:ILE:HD11	1:B:64:LEU:HD21	1.93	0.50
1:B:109:ARG:HD3	1:B:120:LEU:CD2	2.42	0.50
1:A:85:THR:HG21	1:A:184:ARG:CD	2.27	0.49
1:E:101:MET:C	1:E:102:ILE:HD12	2.36	0.49
1:D:19:ILE:HG23	1:D:43:LEU:CD1	2.43	0.49
1:D:82:ASP:CG	1:D:85:THR:HB	2.36	0.49
1:C:46:ILE:HG22	1:C:50:GLY:HA2	1.94	0.49
1:E:39:ARG:O	1:E:40:ASN:HB2	2.11	0.49
1:E:164:GLY:O	1:E:165:LYS:HB2	2.13	0.49
1:A:14:LYS:HB2	1:A:54:GLU:OE2	2.13	0.49
1:A:109:ARG:NH1	1:A:120:LEU:HD21	2.28	0.49
1:A:9:SER:HB3	1:A:83:PRO:HB3	1.94	0.48
1:A:30:SER:HB3	1:D:86:MET:HE3	1.95	0.48
1:E:140:LYS:HE2	1:E:148:ASP:OD1	2.14	0.48
1:D:41:THR:CG2	2:D:191:HOH:O	2.60	0.48
1:B:109:ARG:HD3	1:B:120:LEU:HD23	1.95	0.48
1:B:164:GLY:O	1:B:165:LYS:HB2	2.13	0.48
1:D:36:ILE:CG2	1:D:41:THR:HG21	2.44	0.48
1:B:140:LYS:NZ	1:B:148:ASP:OD1	2.47	0.48
1:C:109:ARG:NH1	1:C:118:SER:OG	2.46	0.48
1:B:109:ARG:CZ	1:B:120:LEU:HD21	2.43	0.47
1:A:140:LYS:HZ1	1:A:148:ASP:CG	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLU:N	2:B:235:HOH:O	2.46	0.47
1:E:103:ASP:C	1:E:105:GLN:H	2.22	0.47
1:E:157:PRO:HB2	2:E:229:HOH:O	2.14	0.47
1:D:136:ARG:HD3	2:D:249:HOH:O	2.15	0.47
1:B:90:THR:HB	1:B:182:LEU:HD11	1.97	0.47
1:A:66:LYS:HB3	1:A:70:GLU:CD	2.40	0.46
1:B:156:MET:HE2	1:C:65:ALA:HB2	1.96	0.46
1:D:82:ASP:OD2	1:D:85:THR:HB	2.15	0.46
1:A:25:LYS:HB2	1:A:38:SER:HB3	1.96	0.46
1:E:36:ILE:HD11	1:E:60:TYR:HA	1.97	0.46
1:E:104:GLY:O	1:E:129:THR:HG23	2.16	0.46
1:B:36:ILE:HD12	1:B:58:VAL:HG11	1.98	0.46
1:D:29:ASN:HB2	1:D:180:ASP:OD1	2.16	0.46
1:A:19:ILE:HG23	1:A:43:LEU:CD1	2.45	0.46
1:C:127:GLU:CD	2:C:217:HOH:O	2.58	0.46
1:E:61:GLY:HA2	1:E:89:ILE:HD12	1.97	0.46
1:B:19:ILE:HG23	1:B:43:LEU:CD1	2.45	0.46
1:A:43:LEU:C	1:A:43:LEU:HD12	2.41	0.46
1:D:101:MET:C	1:D:102:ILE:HD12	2.41	0.46
1:C:139:LEU:HD12	1:C:182:LEU:HB3	1.97	0.46
1:D:76:GLU:OE1	1:E:157:PRO:HG2	2.16	0.46
1:D:102:ILE:HB	1:D:105:GLN:HB3	1.98	0.46
1:A:38:SER:OG	1:A:41:THR:OG1	2.34	0.46
1:B:156:MET:HE1	1:C:78:VAL:C	2.41	0.45
1:E:61:GLY:HA2	1:E:89:ILE:CD1	2.47	0.45
1:A:145:GLN:HB2	1:A:147:ASN:ND2	2.31	0.45
1:A:163:PRO:HD3	2:B:236:HOH:O	2.16	0.45
1:E:13:VAL:CG2	1:E:45:LEU:HD22	2.46	0.45
1:E:98:PHE:HB2	1:E:172:ASP:OD2	2.16	0.45
1:D:95:PHE:HZ	1:E:187:GLN:HG3	1.81	0.45
1:A:90:THR:HG21	1:A:176:ILE:HD12	1.98	0.45
1:B:12:GLN:NE2	2:B:224:HOH:O	2.42	0.45
1:C:19:ILE:HD12	1:C:43:LEU:HD11	1.99	0.45
1:B:19:ILE:HD12	1:B:43:LEU:HD11	1.99	0.45
1:C:36:ILE:HD12	1:C:36:ILE:C	2.41	0.45
1:A:36:ILE:CD1	1:A:58:VAL:HG11	2.47	0.45
1:A:175:GLN:NE2	2:A:213:HOH:O	2.48	0.45
1:E:36:ILE:HD12	1:E:36:ILE:C	2.42	0.45
1:A:83:PRO:O	1:A:187:GLN:NE2	2.50	0.44
1:E:27:VAL:HG21	1:E:178:SER:CB	2.44	0.44
1:D:54:GLU:HB3	1:D:56:TYR:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ILE:HD12	1:E:176:ILE:O	2.16	0.44
1:A:13:VAL:HG12	1:A:76:GLU:O	2.17	0.44
1:B:23:ASN:HA	1:C:117:LEU:HD23	1.99	0.44
1:D:8:GLU:HA	2:D:264:HOH:O	2.16	0.44
1:E:144:ALA:HB3	1:E:145:GLN:HE22	1.83	0.44
1:A:161:PHE:O	1:B:32:GLY:HA2	2.18	0.44
1:E:139:LEU:HD12	1:E:182:LEU:HB3	2.00	0.44
1:A:12:GLN:HG3	1:A:75:GLY:O	2.18	0.43
1:B:176:ILE:C	1:B:176:ILE:HD12	2.43	0.43
1:D:54:GLU:HA	1:D:54:GLU:OE1	2.18	0.43
1:C:152:PRO:HB3	2:C:281:HOH:O	2.19	0.43
1:B:98:PHE:CB	1:B:101:MET:HE3	2.48	0.43
1:E:112:ASP:HB2	1:E:115:THR:CB	2.49	0.43
1:D:114:LEU:H	1:D:114:LEU:CD2	2.25	0.43
1:A:170:LEU:HD13	1:A:176:ILE:CG2	2.47	0.43
1:B:170:LEU:HD12	1:B:170:LEU:O	2.18	0.42
1:D:101:MET:CE	1:D:139:LEU:HD23	2.42	0.42
1:D:112:ASP:O	1:D:114:LEU:HD23	2.19	0.42
1:D:47:ASP:HB3	1:D:53:LYS:HD2	1.99	0.42
1:E:43:LEU:C	1:E:43:LEU:CD1	2.93	0.42
1:E:110:GLN:NE2	1:E:121:VAL:HB	2.34	0.42
1:A:189:SER:O	1:B:145:GLN:NE2	2.52	0.42
1:D:38:SER:OG	1:D:41:THR:HG22	2.20	0.42
1:E:58:VAL:HA	1:E:59:PRO:HD3	1.76	0.42
1:E:90:THR:HB	1:E:182:LEU:HD11	2.01	0.42
1:C:80:ASN:ND2	1:C:81:TRP:H	2.17	0.42
1:A:92:VAL:HG23	1:A:141:ILE:HG21	2.01	0.42
1:D:95:PHE:CE2	1:D:175:GLN:HB2	2.54	0.42
1:A:126:ALA:O	1:A:128:ARG:N	2.52	0.42
1:E:96:VAL:HG23	1:E:176:ILE:HG12	2.01	0.42
1:E:109:ARG:HD2	1:E:118:SER:OG	2.19	0.42
1:C:20:LYS:HD2	1:C:20:LYS:HA	1.75	0.41
1:E:13:VAL:CG2	1:E:45:LEU:HD13	2.46	0.41
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.87	0.41
1:B:175:GLN:NE2	2:B:216:HOH:O	2.47	0.41
1:D:138:ALA:CB	1:D:161:PHE:HA	2.50	0.41
1:E:110:GLN:O	1:E:118:SER:HA	2.21	0.41
1:C:19:ILE:HG23	1:C:43:LEU:HD13	2.01	0.41
1:D:95:PHE:CZ	1:E:187:GLN:HG3	2.55	0.41
1:D:164:GLY:O	1:D:165:LYS:HB2	2.21	0.41
1:E:171:GLU:O	1:E:174:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:LYS:HD2	1:E:68:ASP:OD2	2.21	0.41
1:E:99:THR:H	1:E:101:MET:HE3	1.86	0.41
1:E:185:ILE:HA	1:E:186:PRO:HD2	1.89	0.41
1:A:46:ILE:CG2	1:A:50:GLY:HA2	2.50	0.41
1:C:86:MET:HB2	1:C:187:GLN:HE21	1.82	0.41
1:D:85:THR:HG23	1:D:86:MET:N	2.34	0.41
1:D:114:LEU:HD21	2:D:238:HOH:O	2.21	0.41
1:E:20:LYS:NZ	2:E:241:HOH:O	2.54	0.41
1:A:4:MET:HE3	1:A:6:ALA:CB	2.35	0.41
1:B:128:ARG:HD2	2:B:277:HOH:O	2.21	0.41
1:D:33:LYS:HA	2:D:220:HOH:O	2.20	0.40
1:B:15:ASN:HA	2:B:244:HOH:O	2.21	0.40
1:A:59:PRO:HG2	1:A:81:TRP:CE2	2.57	0.40
1:C:36:ILE:HD11	1:C:60:TYR:HA	2.03	0.40
1:B:110:GLN:O	1:B:118:SER:HA	2.22	0.40
1:B:19:ILE:HG23	1:B:43:LEU:HD11	2.02	0.40
1:C:187:GLN:HB2	1:C:188:GLU:HG2	2.02	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	187/190 (98%)	179 (96%)	5 (3%)	3 (2%)	7	7
1	B	179/190 (94%)	173 (97%)	6 (3%)	0	100	100
1	C	181/190 (95%)	172 (95%)	8 (4%)	1 (1%)	21	27
1	D	181/190 (95%)	175 (97%)	5 (3%)	1 (1%)	21	27
1	E	186/190 (98%)	174 (94%)	11 (6%)	1 (0%)	24	31
All	All	914/950 (96%)	873 (96%)	35 (4%)	6 (1%)	18	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	GLU
1	A	127	GLU
1	D	113	GLU
1	E	187	GLN
1	A	152	PRO
1	A	126	ALA

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	154/156 (99%)	148 (96%)	6 (4%)	28	43
1	B	151/156 (97%)	145 (96%)	6 (4%)	28	42
1	C	151/156 (97%)	147 (97%)	4 (3%)	40	59
1	D	147/156 (94%)	138 (94%)	9 (6%)	17	24
1	E	150/156 (96%)	146 (97%)	4 (3%)	39	58
All	All	753/780 (96%)	724 (96%)	29 (4%)	28	43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	30	SER
1	A	43	LEU
1	A	48	GLU
1	A	85	THR
1	A	109	ARG
1	B	12	GLN
1	B	13	VAL
1	B	43	LEU
1	B	48	GLU
1	B	86	MET
1	B	156	MET

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Mol	Chain	Res	Type
1	C	36	ILE
1	C	43	LEU
1	C	123	LEU
1	C	188	GLU
1	D	16	LYS
1	D	41	THR
1	D	43	LEU
1	D	57	LYS
1	D	85	THR
1	D	114	LEU
1	D	124	ASP
1	D	134	ASP
1	D	188	GLU
1	E	36	ILE
1	E	43	LEU
1	E	176	ILE
1	E	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	147	ASN
1	A	159	GLN
1	A	175	GLN
1	B	12	GLN
1	B	145	GLN
1	B	159	GLN
1	B	175	GLN
1	C	80	ASN
1	C	110	GLN
1	C	169	GLN
1	C	175	GLN
1	D	15	ASN
1	D	84	HIS
1	D	105	GLN
1	D	159	GLN
1	E	15	ASN
1	E	71	GLN
1	E	80	ASN
1	E	84	HIS
1	E	145	GLN

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Mol	Chain	Res	Type
1	E	159	GLN
1	E	169	GLN
1	E	175	GLN
1	E	187	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	189/190 (99%)	0.26	11 (5%) 29 31	14, 31, 58, 73	0
1	B	181/190 (95%)	0.07	6 (3%) 49 51	12, 25, 50, 76	0
1	C	183/190 (96%)	0.45	7 (3%) 44 46	15, 35, 56, 73	0
1	D	183/190 (96%)	0.80	28 (15%) 5 6	18, 36, 80, 90	0
1	E	188/190 (98%)	0.82	26 (13%) 6 7	17, 39, 83, 95	0
All	All	924/950 (97%)	0.48	78 (8%) 17 18	12, 34, 71, 95	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	5.6
1	D	113	GLU	5.4
1	E	114	LEU	5.3
1	E	2	SER	5.0
1	D	115	THR	5.0
1	E	127	GLU	4.9
1	C	7	ALA	4.6
1	D	114	LEU	4.5
1	D	116	GLY	4.4
1	A	1	GLY	4.3
1	D	49	PHE	4.3
1	E	129	THR	4.0
1	D	118	SER	4.0
1	D	117	LEU	3.8
1	A	155	ASP	3.8
1	E	130	ALA	3.8
1	E	117	LEU	3.8
1	D	134	ASP	3.7
1	E	189	SER	3.6
1	E	115	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	ALA	3.5
1	E	131	GLY	3.4
1	D	19	ILE	3.3
1	E	188	GLU	3.3
1	E	169	GLN	3.3
1	A	156	MET	3.2
1	E	108	THR	3.2
1	A	2	SER	3.2
1	B	114	LEU	3.2
1	D	129	THR	3.2
1	B	188	GLU	3.0
1	D	119	SER	2.9
1	D	109	ARG	2.9
1	C	189	SER	2.8
1	E	110	GLN	2.8
1	D	13	VAL	2.8
1	C	9	SER	2.8
1	D	189	SER	2.8
1	E	111	THR	2.8
1	D	127	GLU	2.8
1	D	155	ASP	2.7
1	D	131	GLY	2.7
1	C	188	GLU	2.6
1	D	74	GLY	2.6
1	D	110	GLN	2.6
1	B	113	GLU	2.6
1	E	126	ALA	2.6
1	B	110	GLN	2.5
1	D	7	ALA	2.5
1	E	132	GLY	2.5
1	D	169	GLN	2.4
1	D	130	ALA	2.4
1	E	187	GLN	2.4
1	C	49	PHE	2.4
1	E	128	ARG	2.4
1	A	125	SER	2.3
1	D	14	LYS	2.3
1	A	114	LEU	2.3
1	A	4	MET	2.3
1	B	115	THR	2.3
1	E	3	HIS	2.3
1	E	153	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	71	GLN	2.2
1	E	84	HIS	2.2
1	E	40	ASN	2.2
1	E	112	ASP	2.2
1	E	116	GLY	2.2
1	A	150	LEU	2.2
1	B	116	GLY	2.2
1	E	113	GLU	2.1
1	A	5	ALA	2.1
1	C	113	GLU	2.1
1	D	125	SER	2.0
1	D	48	GLU	2.0
1	A	12	GLN	2.0
1	E	121	VAL	2.0
1	D	50	GLY	2.0
1	D	53	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.