



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:24 AM GMT

PDB ID : 2FEC
Title : Structure of the E203Q mutant of the Cl⁻/H⁺ exchanger CLC-ec1 from E.Coli
Authors : Accardi, A.; Walden, M.P.; Nguitragool, W.; Jayaram, H.; Williams, C.;
Miller, C.
Deposited on : 2005-12-15
Resolution : 3.97 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

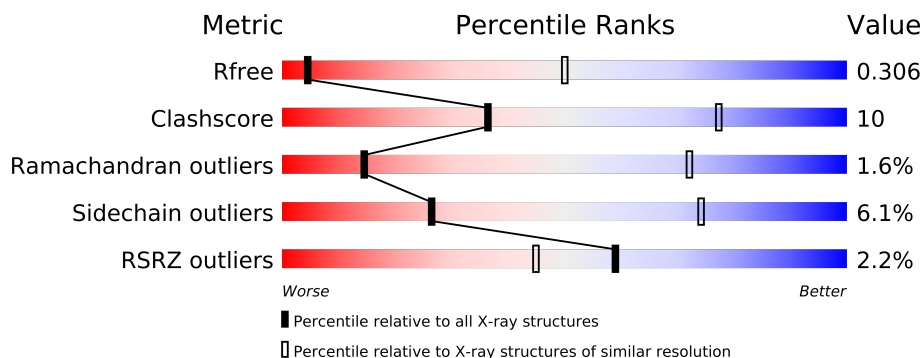
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.97 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}	66092	1005 (4.46-3.46)
Clashscore	79885	1195 (4.42-3.50)
Ramachandran outliers	78287	1137 (4.42-3.50)
Sidechain outliers	78261	1124 (4.42-3.50)
RSRZ outliers	66119	1005 (4.46-3.46)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	465	
1	B	465	
2	I	222	
2	J	222	
3	L	211	
3	O	211	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13223 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	561	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	554	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLN	GLU	ENGINEERED	UNP P37019
B	203	GLN	GLU	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	I	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab fragment, light chain.

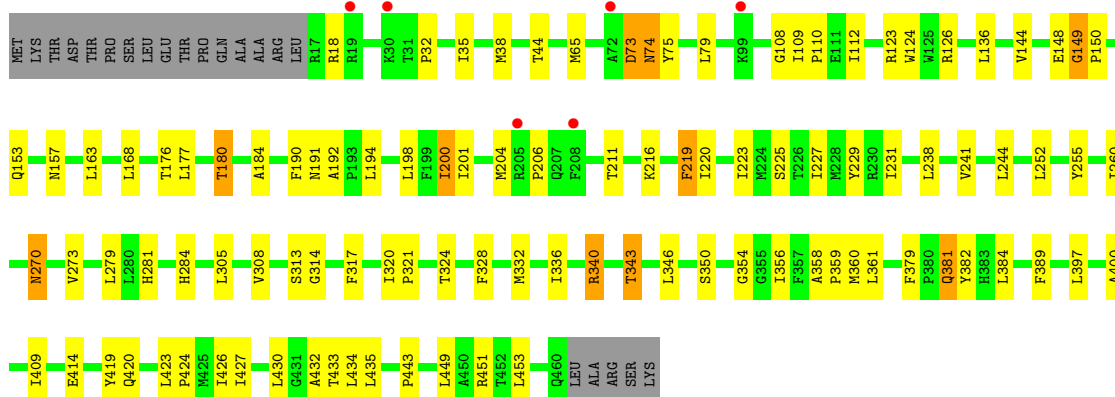
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	L	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

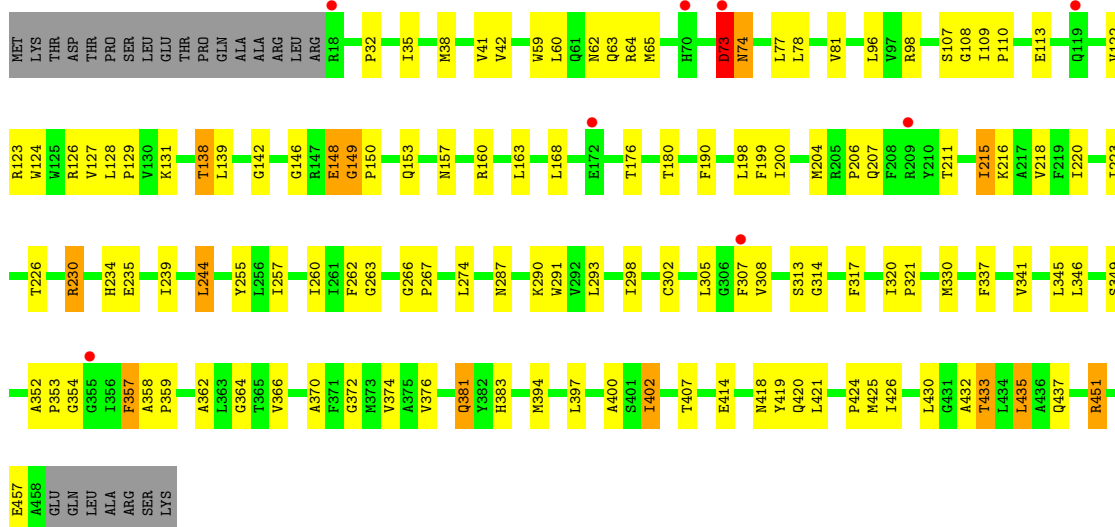
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain A: 



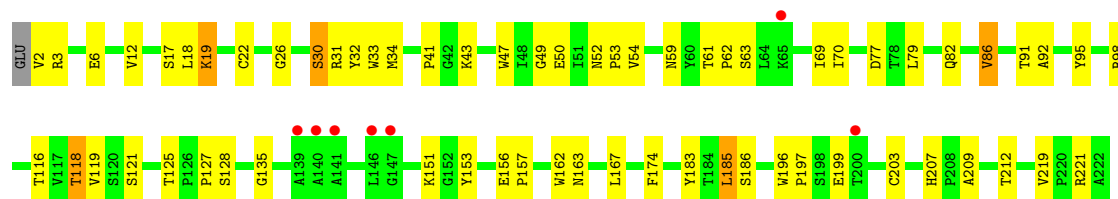
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain B: 



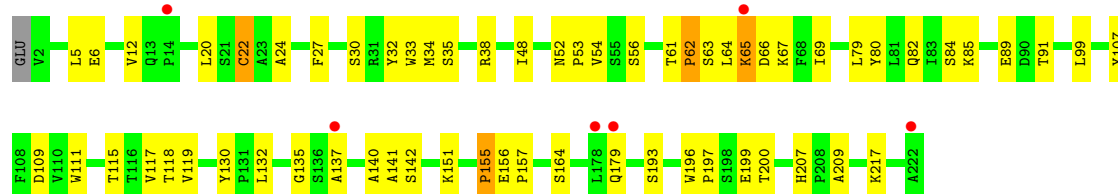
- Molecule 2: Fab fragment, heavy chain

Chain J: 



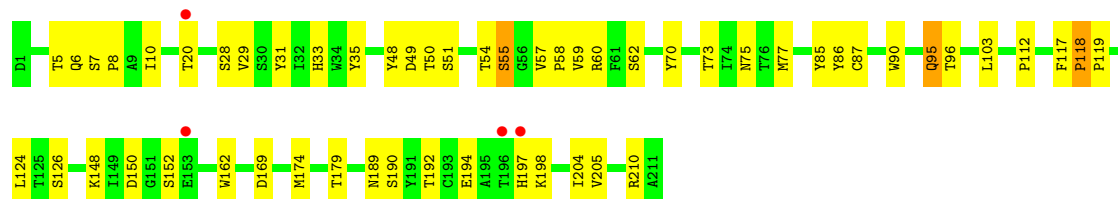
• Molecule 2: Fab fragment, heavy chain

Chain I:



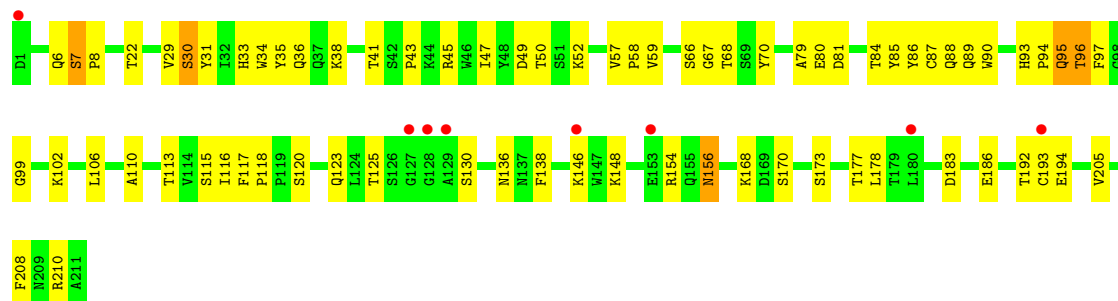
• Molecule 3: Fab fragment, light chain

Chain O:



• Molecule 3: Fab fragment, light chain

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.31Å 98.50Å 170.41Å 90.00° 131.51° 90.00°	Depositor
Resolution (Å)	128.04 – 3.97 33.31 – 3.97	Depositor EDS
% Data completeness (in resolution range)	97.8 (128.04-3.97) 97.9 (33.31-3.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.269 , 0.326 0.255 , 0.306	Depositor DCC
R_{free} test set	1258 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	141.0	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 78.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24578 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.43	0/3405	0.53	0/4621
1	B	0.49	1/3376 (0.0%)	0.55	0/4583
2	I	0.40	0/1721	0.55	0/2355
2	J	0.72	4/1721 (0.2%)	0.59	2/2355 (0.1%)
3	L	0.38	0/1660	0.54	0/2257
3	O	0.42	0/1660	0.52	0/2257
All	All	0.48	5/13543 (0.0%)	0.55	2/18428 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	19	LYS	CE-NZ	13.79	1.83	1.49
2	J	199	GLU	CD-OE2	13.32	1.40	1.25
2	J	199	GLU	CD-OE1	12.20	1.39	1.25
1	B	73	ASP	C-O	10.60	1.43	1.23
2	J	19	LYS	CD-CE	8.95	1.73	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	19	LYS	CD-CE-NZ	-7.37	94.75	111.70
2	J	185	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3486	63	0
1	B	3304	0	3459	86	0
2	I	1672	0	1654	34	0
2	J	1672	0	1654	35	0
3	L	1621	0	1546	47	0
3	O	1621	0	1546	30	0
All	All	13223	0	13345	273	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (273) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:19:LYS:CE	2:J:19:LYS:NZ	1.83	1.41
3:L:7:SER:HB3	3:L:8:PRO:HD3	1.41	1.00
3:L:146:LYS:HB3	3:L:194:GLU:HB2	1.44	1.00
1:B:381:GLN:HE21	1:B:381:GLN:H	1.15	0.92
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.59	0.84
3:O:6:GLN:HE22	3:O:86:TYR:HA	1.52	0.74
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.69	0.74
1:A:381:GLN:NE2	1:A:381:GLN:H	1.85	0.74
1:B:381:GLN:N	1:B:381:GLN:HE21	1.86	0.72
1:B:148:GLU:CD	1:B:148:GLU:H	1.93	0.72
3:L:7:SER:CB	3:L:8:PRO:HD3	2.19	0.72
3:L:36:GLN:HG3	3:L:85:TYR:CE2	2.25	0.71
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.73	0.70
1:B:381:GLN:NE2	1:B:381:GLN:H	1.88	0.69
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.75	0.69
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.75	0.69
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.75	0.68
3:O:148:LYS:HB2	3:O:192:THR:OG1	1.95	0.67
2:J:91:THR:HG23	2:J:118:THR:HA	1.76	0.66
3:L:6:GLN:HG3	3:L:99:GLY:H	1.61	0.66
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.78	0.65
1:A:227:ILE:O	1:A:231:ILE:HG12	1.97	0.64
3:L:34:TRP:HB2	3:L:47:ILE:HB	1.80	0.64
1:A:144:VAL:HG21	1:A:343:THR:HB	1.80	0.64
3:O:29:VAL:HG23	3:O:70:TYR:HE1	1.63	0.63
2:J:207:HIS:CE1	2:J:209:ALA:HB3	2.35	0.62
2:I:130:TYR:HB3	3:L:120:SER:OG	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:19:LYS:CD	2:J:19:LYS:NZ	2.62	0.62
2:J:156:GLU:OE1	2:J:157:PRO:HA	2.00	0.62
3:L:7:SER:HB2	3:L:22:THR:HB	1.81	0.61
2:I:91:THR:HA	2:I:117:VAL:O	2.00	0.61
2:J:33:TRP:CZ2	2:J:52:ASN:HB3	2.35	0.61
1:A:148:GLU:H	1:A:148:GLU:CD	2.03	0.61
1:A:384:LEU:HD22	1:A:389:PHE:HE1	1.64	0.60
1:B:298:ILE:HG12	1:B:346:LEU:HD23	1.84	0.60
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.84	0.60
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.67	0.60
3:L:7:SER:HB3	3:L:8:PRO:CD	2.24	0.59
1:B:176:THR:O	1:B:180:THR:HG23	2.02	0.59
2:I:91:THR:HG23	2:I:118:THR:HA	1.84	0.59
1:B:113:GLU:HG3	1:B:204:MET:SD	2.42	0.59
1:B:180:THR:HG22	1:B:218:VAL:HA	1.84	0.59
3:O:194:GLU:HG2	3:O:205:VAL:HG12	1.84	0.59
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.85	0.59
3:L:88:GLN:HB2	3:L:97:PHE:CD1	2.38	0.59
3:L:194:GLU:HG2	3:L:205:VAL:HG12	1.83	0.58
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.85	0.58
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.86	0.58
1:A:313:SER:OG	1:A:314:GLY:N	2.36	0.58
1:A:409:ILE:HD13	1:A:426:ILE:HA	1.86	0.58
3:L:38:LYS:O	3:L:41:THR:HG22	2.04	0.58
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.85	0.58
1:B:239:ILE:HD13	1:B:394:MET:HE1	1.86	0.58
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.85	0.57
2:I:91:THR:OG1	2:I:119:VAL:HG23	2.04	0.57
1:A:176:THR:O	1:A:180:THR:HG23	2.05	0.57
1:B:362:ALA:O	1:B:366:VAL:HG23	2.04	0.57
3:L:136:ASN:HD22	3:L:173:SER:HB3	1.68	0.57
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.86	0.57
3:L:31:TYR:HA	3:L:50:THR:OG1	2.04	0.56
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.86	0.56
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.88	0.56
3:L:146:LYS:HB3	3:L:194:GLU:CB	2.29	0.56
1:B:38:MET:HA	1:B:41:VAL:HG12	1.86	0.56
2:I:69:ILE:HB	2:I:82:GLN:HB2	1.87	0.56
3:L:66:SER:HA	3:L:70:TYR:CZ	2.41	0.56
3:L:89:GLN:HE21	3:L:96:THR:H	1.52	0.56
2:I:24:ALA:HB1	2:I:27:PHE:CE1	2.40	0.55
3:L:93:HIS:CG	3:L:94:PRO:HA	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:O:124:LEU:C	3:O:126:SER:H	2.10	0.55
3:O:6:GLN:NE2	3:O:87:CYS:H	2.04	0.55
2:J:61:THR:O	2:J:63:SER:N	2.40	0.55
1:B:59:TRP:O	1:B:63:GLN:HG2	2.08	0.54
2:I:141:ALA:O	2:I:193:SER:HB2	2.08	0.54
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.89	0.54
1:B:402:ILE:HG13	1:B:402:ILE:O	2.05	0.54
2:J:127:PRO:HD2	2:J:212:THR:HG21	1.89	0.53
1:A:194:LEU:CD2	1:B:426:ILE:HD11	2.39	0.53
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.91	0.53
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.73	0.53
3:L:115:SER:HB3	3:L:117:PHE:HE1	1.74	0.53
1:A:112:ILE:HD11	1:A:153:GLN:HG3	1.91	0.53
3:O:31:TYR:HA	3:O:50:THR:OG1	2.08	0.53
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.90	0.53
2:J:6:GLU:HA	2:J:22:CYS:HA	1.90	0.53
3:O:95:GLN:CD	3:O:95:GLN:N	2.63	0.52
2:I:84:SER:HB3	2:I:85:LYS:HE2	1.91	0.52
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.74	0.52
1:A:414:GLU:HG2	1:B:419:TYR:CE1	2.44	0.52
2:J:49:GLY:HA3	2:J:70:ILE:HD12	1.90	0.52
3:O:31:TYR:HB3	3:O:49:ASP:OD1	2.09	0.52
1:B:274:LEU:HB3	1:B:451:ARG:NH2	2.24	0.52
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.91	0.52
3:L:29:VAL:HG23	3:L:70:TYR:CE1	2.45	0.52
2:J:33:TRP:CH2	2:J:52:ASN:HB3	2.45	0.52
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.90	0.52
2:I:207:HIS:CE1	2:I:209:ALA:HB3	2.45	0.52
2:I:61:THR:OG1	2:I:62:PRO:HD2	2.09	0.52
2:I:63:SER:OG	2:I:64:LEU:N	2.43	0.51
2:J:30:SER:C	2:J:32:TYR:H	2.14	0.51
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.39	0.51
3:L:36:GLN:O	3:L:43:PRO:HA	2.11	0.51
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.91	0.51
1:B:337:PHE:O	1:B:341:VAL:HG23	2.11	0.51
3:O:95:GLN:CD	3:O:95:GLN:H	2.13	0.51
1:A:336:ILE:O	1:A:340:ARG:HG3	2.09	0.51
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.46	0.51
2:J:69:ILE:HB	2:J:82:GLN:HB2	1.92	0.50
3:O:90:TRP:CG	3:O:95:GLN:HB3	2.47	0.50
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.75	0.50
3:L:30:SER:HA	3:L:70:TYR:OH	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:49:GLY:HA3	2:J:70:ILE:CD1	2.42	0.50
2:I:107:TYR:HB3	3:L:33:HIS:CD2	2.47	0.50
3:L:6:GLN:NE2	3:L:87:CYS:H	2.09	0.50
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.93	0.50
3:L:79:ALA:C	3:L:81:ASP:H	2.15	0.50
1:A:73:ASP:O	1:A:74:ASN:C	2.50	0.50
3:O:189:ASN:HD22	3:O:210:ARG:HB2	1.77	0.50
3:L:186:GLU:HG2	3:L:210:ARG:NH1	2.27	0.50
3:L:7:SER:CB	3:L:8:PRO:CD	2.89	0.49
3:O:162:TRP:CD1	3:O:174:MET:HG3	2.46	0.49
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.94	0.49
3:L:115:SER:HB3	3:L:117:PHE:CE1	2.48	0.49
3:L:115:SER:CB	3:L:117:PHE:HE1	2.25	0.49
1:B:32:PRO:HD2	1:B:35:ILE:HD12	1.94	0.49
2:I:109:ASP:HA	3:L:45:ARG:HD3	1.94	0.49
2:J:163:ASN:HD22	2:J:167:LEU:HB2	1.77	0.49
1:B:287:ASN:HD22	1:B:290:LYS:H	1.59	0.49
2:I:34:MET:HB3	2:I:79:LEU:HD22	1.95	0.49
1:B:421:LEU:O	1:B:425:MET:HG3	2.12	0.48
3:L:123:GLN:NE2	3:L:130:SER:H	2.10	0.48
2:I:52:ASN:HD21	2:I:56:SER:H	1.61	0.48
2:J:207:HIS:HE1	2:J:209:ALA:HB3	1.76	0.48
1:A:108:GLY:O	1:A:112:ILE:HG12	2.13	0.48
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.95	0.48
2:I:61:THR:O	2:I:63:SER:N	2.47	0.48
1:B:257:ILE:HA	1:B:260:ILE:HD12	1.95	0.48
3:O:197:HIS:CG	3:O:198:LYS:H	2.32	0.48
3:L:110:ALA:O	3:L:138:PHE:HA	2.14	0.48
1:B:370:ALA:O	1:B:374:VAL:HG23	2.14	0.48
3:O:60:ARG:HB2	3:O:75:ASN:O	2.13	0.48
3:L:95:GLN:N	3:L:95:GLN:CD	2.68	0.48
1:A:252:LEU:HD22	1:A:427:ILE:HD12	1.95	0.48
3:L:118:PRO:HB3	3:L:208:PHE:CE1	2.48	0.47
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.44	0.47
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.95	0.47
1:A:419:TYR:CE1	1:B:414:GLU:HG2	2.49	0.47
1:B:148:GLU:HG3	1:B:190:PHE:CZ	2.49	0.47
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.49	0.47
2:I:6:GLU:HA	2:I:22:CYS:HA	1.96	0.47
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.50	0.47
2:I:38:ARG:HG2	2:I:48:ILE:HD11	1.96	0.47
1:B:148:GLU:OE2	1:B:358:ALA:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:41:PRO:HD3	2:J:92:ALA:HA	1.96	0.47
2:I:52:ASN:HB2	2:I:53:PRO:CD	2.45	0.47
1:A:346:LEU:O	1:A:350:SER:HB3	2.14	0.47
2:J:49:GLY:HA2	2:J:59:ASN:O	2.14	0.47
2:J:174:PHE:HD2	2:J:186:SER:O	1.97	0.47
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.97	0.47
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.95	0.47
1:A:384:LEU:HD22	1:A:389:PHE:CE1	2.49	0.47
1:B:73:ASP:O	1:B:74:ASN:C	2.53	0.47
3:O:148:LYS:HA	3:O:152:SER:O	2.15	0.47
1:B:305:LEU:C	1:B:307:PHE:H	2.17	0.47
2:J:127:PRO:HB3	2:J:153:TYR:HB3	1.97	0.47
1:A:109:ILE:N	1:A:110:PRO:CD	2.77	0.47
2:J:47:TRP:HZ2	2:J:50:GLU:HG2	1.79	0.47
2:I:111:TRP:HE1	3:L:35:TYR:HE2	1.63	0.47
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.50	0.47
1:A:148:GLU:O	1:A:149:GLY:C	2.53	0.46
2:I:24:ALA:HB1	2:I:27:PHE:HE1	1.80	0.46
3:O:77:MET:SD	3:O:103:LEU:HD21	2.56	0.46
2:J:2:VAL:HA	2:J:26:GLY:HA3	1.97	0.46
1:B:38:MET:O	1:B:42:VAL:HG23	2.15	0.46
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.64	0.46
3:L:130:SER:HA	3:L:178:LEU:O	2.16	0.46
3:L:123:GLN:HE22	3:L:130:SER:H	1.63	0.46
3:L:148:LYS:HB2	3:L:192:THR:OG1	2.15	0.46
3:L:90:TRP:CD2	3:L:95:GLN:HB3	2.50	0.46
1:B:263:GLY:O	1:B:267:PRO:HD3	2.16	0.46
1:B:230:ARG:O	1:B:234:HIS:HB3	2.16	0.46
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.97	0.46
1:A:358:ALA:HA	1:A:361:LEU:HD12	1.98	0.46
1:B:60:LEU:O	1:B:64:ARG:HG3	2.17	0.45
1:A:194:LEU:HD21	1:B:426:ILE:HD11	1.97	0.45
1:B:109:ILE:N	1:B:110:PRO:CD	2.79	0.45
2:J:196:TRP:CG	2:J:197:PRO:HA	2.50	0.45
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.45
1:B:313:SER:OG	1:B:314:GLY:N	2.50	0.45
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	0.45
1:A:381:GLN:N	1:A:381:GLN:NE2	2.62	0.45
2:J:33:TRP:CE2	2:J:52:ASN:HB3	2.52	0.45
3:O:197:HIS:CG	3:O:198:LYS:N	2.85	0.45
2:I:65:LYS:HB2	2:I:66:ASP:H	1.65	0.45
1:B:190:PHE:CE2	1:B:317:PHE:HZ	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:20:LEU:O	2:I:80:TYR:HA	2.17	0.44
1:B:320:ILE:HB	1:B:321:PRO:HD3	2.00	0.44
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.81	0.44
1:B:215:ILE:H	1:B:215:ILE:HG13	1.51	0.44
2:I:200:THR:HG23	2:I:217:LYS:HE3	1.98	0.44
1:B:383:HIS:HD2	2:I:33:TRP:CZ3	2.36	0.44
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.53	0.44
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.99	0.44
2:J:52:ASN:HB2	2:J:53:PRO:HD2	2.00	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.18	0.44
3:O:35:TYR:O	3:O:85:TYR:HA	2.18	0.44
1:B:180:THR:CG2	1:B:218:VAL:HA	2.48	0.43
2:I:65:LYS:H	2:I:65:LYS:HG3	1.52	0.43
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.53	0.43
1:B:142:GLY:O	1:B:302:CYS:HB3	2.18	0.43
3:L:49:ASP:HB2	3:L:52:LYS:HD2	2.00	0.43
2:I:196:TRP:CG	2:I:197:PRO:HA	2.52	0.43
2:I:155:PRO:HB2	2:I:156:GLU:H	1.70	0.43
1:B:78:LEU:HA	1:B:81:VAL:HG22	2.01	0.43
2:J:163:ASN:HD21	2:J:167:LEU:HD22	1.82	0.43
1:B:345:LEU:O	1:B:349:SER:HB2	2.17	0.43
2:J:86:VAL:HG12	2:J:119:VAL:HG21	2.01	0.43
3:L:57:VAL:HA	3:L:58:PRO:HD2	1.86	0.43
3:L:116:ILE:HD13	3:L:193:CYS:HB2	2.01	0.43
3:O:150:ASP:HA	3:O:190:SER:HB3	2.01	0.43
3:O:117:PHE:HA	3:O:118:PRO:HD3	1.92	0.43
1:B:199:PHE:HA	1:B:407:THR:OG1	2.19	0.43
1:B:148:GLU:O	1:B:149:GLY:C	2.57	0.42
1:B:234:HIS:HD1	1:B:235:GLU:HG2	1.84	0.42
1:B:266:GLY:HA3	1:B:400:ALA:HB1	2.01	0.42
3:L:154:ARG:HH21	3:L:156:ASN:HB2	1.84	0.42
1:A:241:VAL:HG11	1:A:324:THR:HG21	2.01	0.42
1:A:356:ILE:O	1:A:360:MET:HG3	2.19	0.42
1:A:328:PHE:HD1	1:A:332:MET:HG2	1.84	0.42
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.84	0.42
3:O:62:SER:OG	3:O:73:THR:HB	2.19	0.42
1:B:148:GLU:CD	1:B:148:GLU:N	2.68	0.42
2:I:132:LEU:HB3	3:L:117:PHE:CD2	2.54	0.42
1:A:32:PRO:HD2	1:A:35:ILE:HD12	2.01	0.42
3:O:112:PRO:HG2	3:O:204:ILE:HD12	2.01	0.42
3:O:33:HIS:ND1	3:O:48:TYR:HB2	2.35	0.42
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.35	0.42
3:O:54:THR:HG22	3:O:55:SER:N	2.35	0.42
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.35	0.42
2:J:12:VAL:HG11	2:J:18:LEU:HD22	2.01	0.42
1:B:330:MET:O	1:B:330:MET:HE2	2.19	0.42
2:J:156:GLU:HG2	2:J:183:TYR:CE1	2.55	0.41
2:J:30:SER:O	2:J:32:TYR:N	2.53	0.41
2:I:30:SER:C	2:I:32:TYR:H	2.23	0.41
1:B:108:GLY:H	1:B:110:PRO:HD2	1.85	0.41
2:J:196:TRP:CD1	2:J:197:PRO:HA	2.55	0.41
2:I:67:LYS:HD2	2:I:67:LYS:HA	1.89	0.41
1:B:131:LYS:HD3	1:B:153:GLN:NE2	2.35	0.41
3:L:117:PHE:HA	3:L:118:PRO:HD3	1.76	0.41
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.20	0.41
3:O:58:PRO:HB2	3:O:60:ARG:HG2	2.02	0.41
1:B:122:VAL:HB	1:B:160:ARG:HG2	2.03	0.41
1:A:194:LEU:HD23	1:B:426:ILE:HD11	2.01	0.41
2:I:35:SER:HB2	2:I:99:LEU:HD11	2.01	0.41
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.56	0.41
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.03	0.41
2:J:162:TRP:CZ3	2:J:203:CYS:HB3	2.55	0.41
2:I:135:GLY:C	2:I:137:ALA:H	2.23	0.41
1:A:216:LYS:HE2	1:B:433:THR:HG22	2.02	0.41
3:L:93:HIS:ND1	3:L:94:PRO:HA	2.36	0.40
1:B:372:GLY:O	1:B:376:VAL:HG23	2.21	0.40
1:B:244:LEU:HB2	1:B:418:ASN:OD1	2.20	0.40
2:I:89:GLU:OE1	2:I:89:GLU:N	2.54	0.40
3:O:29:VAL:HG23	3:O:70:TYR:CE1	2.50	0.40
1:B:200:ILE:HA	1:B:204:MET:HB2	2.03	0.40
1:B:138:THR:HG21	1:B:352:ALA:HB1	2.03	0.40
3:O:118:PRO:HA	3:O:119:PRO:HD2	1.96	0.40
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.22	0.40
2:J:6:GLU:OE2	2:J:95:TYR:HA	2.21	0.40
3:O:57:VAL:HA	3:O:58:PRO:HD2	1.87	0.40
2:J:135:GLY:HA2	2:J:221:ARG:HE	1.87	0.40
3:O:7:SER:HB3	3:O:8:PRO:HD3	2.03	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	442/465 (95%)	411 (93%)	25 (6%)	6 (1%)	16	74
1	B	439/465 (94%)	406 (92%)	29 (7%)	4 (1%)	25	81
2	I	219/222 (99%)	192 (88%)	20 (9%)	7 (3%)	6	57
2	J	219/222 (99%)	193 (88%)	24 (11%)	2 (1%)	25	81
3	L	209/211 (99%)	181 (87%)	22 (10%)	6 (3%)	7	59
3	O	209/211 (99%)	181 (87%)	25 (12%)	3 (1%)	16	74
All	All	1737/1796 (97%)	1564 (90%)	145 (8%)	28 (2%)	14	72

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	B	73	ASP
3	O	55	SER
3	L	7	SER
1	A	74	ASN
1	B	74	ASN
2	J	62	PRO
2	I	62	PRO
2	I	65	LYS
2	J	31	ARG
2	I	140	ALA
3	L	59	VAL
3	L	170	SER
1	A	149	GLY
3	O	51	SER
3	O	169	ASP
2	I	142	SER
3	L	80	GLU
3	L	102	LYS
1	B	149	GLY
2	I	164	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	67	GLY
1	A	206	PRO
1	B	206	PRO
1	A	443	PRO
1	A	201	ILE
2	I	155	PRO
2	I	157	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/353 (95%)	317 (95%)	18 (5%)	31	78
1	B	332/353 (94%)	309 (93%)	23 (7%)	22	69
2	I	181/182 (100%)	173 (96%)	8 (4%)	39	83
2	J	181/182 (100%)	165 (91%)	16 (9%)	14	59
3	L	185/185 (100%)	173 (94%)	12 (6%)	24	72
3	O	185/185 (100%)	176 (95%)	9 (5%)	35	80
All	All	1399/1440 (97%)	1313 (94%)	86 (6%)	26	74

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	65	MET
1	A	136	LEU
1	A	180	THR
1	A	200	ILE
1	A	211	THR
1	A	219	PHE
1	A	238	LEU
1	A	244	LEU
1	A	270	ASN
1	A	279	LEU
1	A	340	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	343	THR
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	451	ARG
1	B	62	ASN
1	B	65	MET
1	B	73	ASP
1	B	96	LEU
1	B	107	SER
1	B	138	THR
1	B	139	LEU
1	B	148	GLU
1	B	207	GLN
1	B	211	THR
1	B	215	ILE
1	B	230	ARG
1	B	244	LEU
1	B	293	LEU
1	B	357	PHE
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	433	THR
1	B	435	LEU
1	B	437	GLN
1	B	451	ARG
2	J	3	ARG
2	J	17	SER
2	J	30	SER
2	J	43	LYS
2	J	54	VAL
2	J	77	ASP
2	J	86	VAL
2	J	98	ARG
2	J	116	THR
2	J	118	THR
2	J	121	SER
2	J	125	THR
2	J	128	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	151	LYS
2	J	185	LEU
2	J	219	VAL
3	O	5	THR
3	O	10	ILE
3	O	20	THR
3	O	28	SER
3	O	59	VAL
3	O	95	GLN
3	O	96	THR
3	O	118	PRO
3	O	179	THR
2	I	5	LEU
2	I	12	VAL
2	I	22	CYS
2	I	54	VAL
2	I	115	THR
2	I	151	LYS
2	I	179	GLN
2	I	199	GLU
3	L	30	SER
3	L	68	THR
3	L	84	THR
3	L	95	GLN
3	L	96	THR
3	L	106	LEU
3	L	113	THR
3	L	125	THR
3	L	156	ASN
3	L	168	LYS
3	L	177	THR
3	L	183	ASP

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

Mol	Chain	Res	Type
1	A	153	GLN
1	A	157	ASN
1	A	207	GLN
1	A	233	ASN
1	A	327	ASN
1	A	381	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	ASN
1	B	62	ASN
1	B	157	ASN
1	B	270	ASN
1	B	287	ASN
1	B	318	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS
2	J	163	ASN
2	J	207	HIS
3	O	6	GLN
3	O	36	GLN
3	O	189	ASN
3	L	6	GLN
3	L	89	GLN
3	L	123	GLN
3	L	136	ASN
3	L	137	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates 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(Å²)	Q<0.9	
1	A	444/465 (95%)	0.15	6 (1%)	72	57	117, 150, 183, 202	0
1	B	441/465 (94%)	0.21	8 (1%)	65	51	121, 158, 194, 210	0
2	I	221/222 (99%)	0.24	6 (2%)	52	40	131, 162, 185, 194	0
2	J	221/222 (99%)	0.29	7 (3%)	45	36	131, 146, 169, 176	0
3	L	211/211 (100%)	0.32	8 (3%)	38	31	115, 139, 188, 197	0
3	O	211/211 (100%)	0.28	4 (1%)	64	49	152, 167, 181, 183	0
All	All	1749/1796 (97%)	0.23	39 (2%)	59	45	115, 156, 185, 210	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	147	GLY	5.4
3	L	128	GLY	3.8
2	J	65	LYS	3.7
3	L	127	GLY	3.3
1	B	355	GLY	3.2
3	O	20	THR	3.1
1	B	18	ARG	3.0
2	J	139	ALA	2.8
1	B	73	ASP	2.7
2	J	200	THR	2.6
3	O	197	HIS	2.6
1	A	72	ALA	2.6
3	O	153	GLU	2.5
2	I	178	LEU	2.5
2	J	146	LEU	2.5
2	I	179	GLN	2.4
1	B	119	GLN	2.4
3	O	196	THR	2.3
1	A	19	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	2.3
2	I	222	ALA	2.3
3	L	1	ASP	2.2
2	J	140	ALA	2.2
3	L	180	LEU	2.2
3	L	153	GLU	2.2
2	J	141	ALA	2.2
1	B	172	GLU	2.2
1	B	209	ARG	2.2
1	B	70	HIS	2.1
1	A	99	LYS	2.1
3	L	193	CYS	2.1
3	L	129	ALA	2.1
2	I	65	LYS	2.1
1	A	208	PHE	2.0
1	A	205	ARG	2.0
2	I	14	PRO	2.0
1	A	30	LYS	2.0
2	I	137	ALA	2.0
3	L	146	LYS	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 carbohydrates 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.