



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:24 AM GMT

PDB ID : 4JW1
Title : Crystal structure of N-terminal 618-residue fragment of LepB from Legionella pneumophila
Authors : Hu, L.; Yao, Q.; Zhu, Y.; Shao, F.
Deposited on : 2013-03-26
Resolution : 3.16 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>

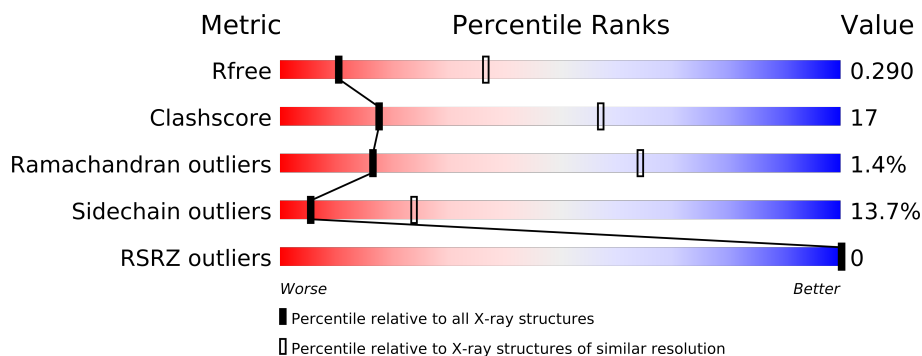
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.16 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	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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	626	
1	B	626	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	701	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6745 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 Effector protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	Se	0	1	0
			4130	2679	676	758	7	10			
1	B	319	Total	C	N	O	S	Se	0	0	0
			2569	1670	426	467	4	2			

There are 22 discrepancies between the modelled and reference sequences:

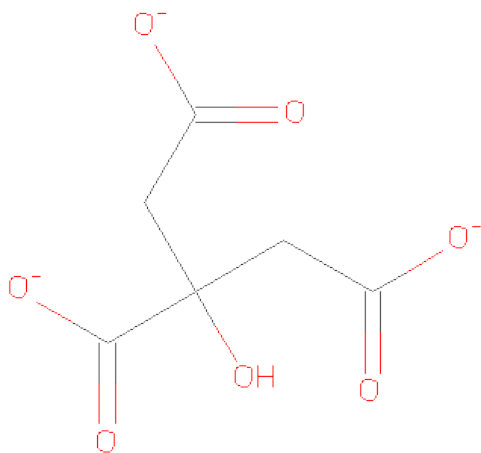
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-6	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-5	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-4	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-3	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-2	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
A	-1	GLY	-	EXPRESSION TAG	UNP Q6X1Y7
A	0	PRO	-	EXPRESSION TAG	UNP Q6X1Y7
A	13	ALA	LYS	CONFLICT	UNP Q6X1Y7
A	14	ALA	GLU	CONFLICT	UNP Q6X1Y7
A	15	ALA	LYS	CONFLICT	UNP Q6X1Y7
B	-7	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-6	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-5	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-4	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-3	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-2	HIS	-	EXPRESSION TAG	UNP Q6X1Y7
B	-1	GLY	-	EXPRESSION TAG	UNP Q6X1Y7
B	0	PRO	-	EXPRESSION TAG	UNP Q6X1Y7
B	13	ALA	LYS	CONFLICT	UNP Q6X1Y7
B	14	ALA	GLU	CONFLICT	UNP Q6X1Y7
B	15	ALA	LYS	CONFLICT	UNP Q6X1Y7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

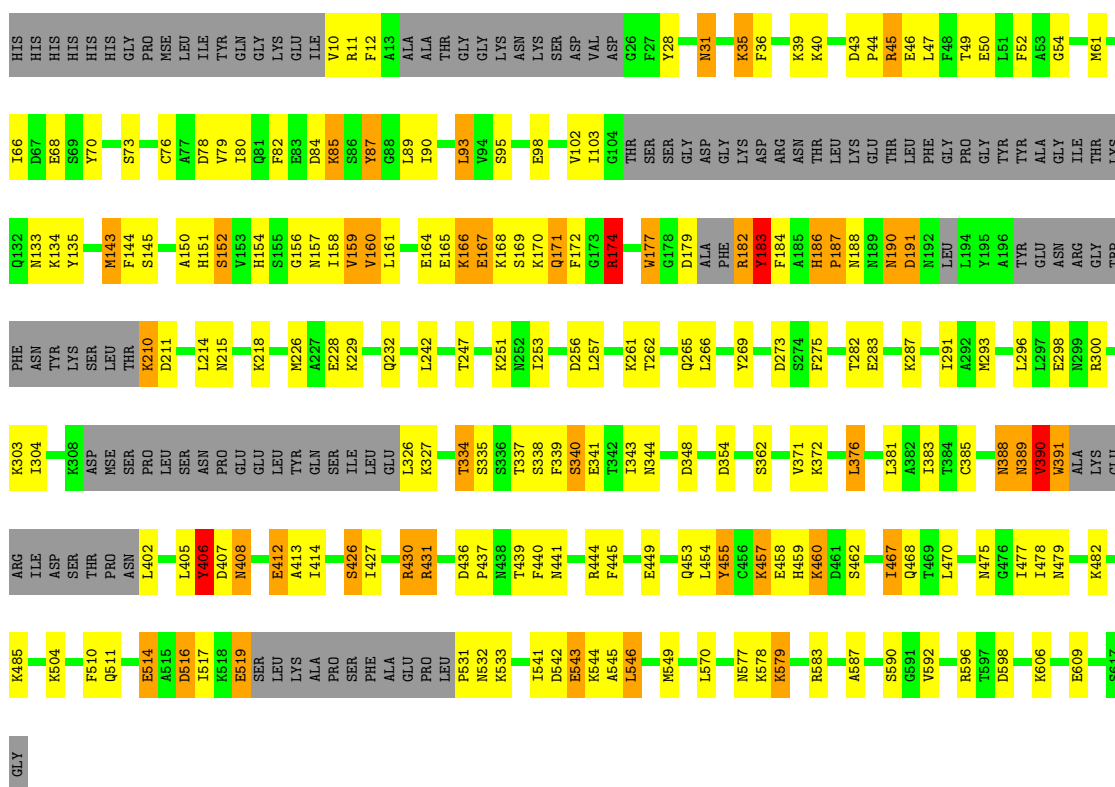
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			1	1		

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.

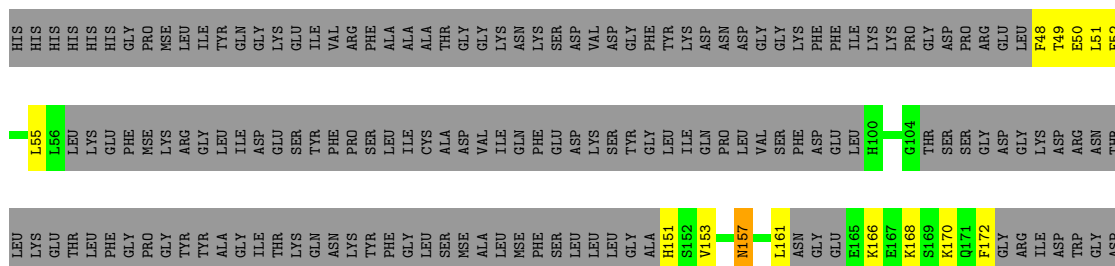
• Molecule 1: Effector protein B

Chain A:



• Molecule 1: Effector protein B

Chain B:



ALA PHE ARG TYR PHE ALA HIS PRO ASN ASN ASN ASP ASN LEU LEU TYR ALA TYR GLU ASN R200 G201 G202 PHE ASN TYR LYS SER LEU THR THR MSE MSE MSE CYS MSE F213 L214 N215 Y216 K217 LYS L219 ASN GLY LEU PHE PRO ALA MSE ALA GLY LYS PHE LYS ALA ARG GLN GLN GLN SER LYS LEU LEU ASN PRO	GLU LEU VAL LYS ILE VAL THR SER ALA L250 K251 N252 I253 P254 A255 D256 L257 ILE ASP GLU LYS THR GLN SER ILE LEU GLN LEU ALA TYR THR MSE MSE MSE CYS ASP SER PHE LYS GLY THR GLY GLY ASN CYS LYS ASP PHE ALA ILE ALA MSE ALA THR GLU LEU GLU ASN	ARG LEU GLY LYS ILE VAL LEU LYS ASP MSE SER PRO LEU SER ASN PRO GLU GLU LEU TYR GLN SER ILE LEU GLU LEU K327 P328 L329 T330 L331 S336 T337 S340 E341 N344 Q345 W346 T349 T352 THR MSE GLU K357 D361 S362 N363 P364 I365 V371 Y422 T425 L429 R430 R431 L432 F433 T434 R444 P445 G450 Q453 L454 K457 E458 H459 K460 D461 S462 V465 N577	N375 D379 I383 E386 V390 W391 A392 LYS E394 ARG ILE ASP SER THR PRO M401 L402 F403 Y406 D407 M408 S409 E412 A413 I414 H415 Y422 T425 L429 R430 R431 L432 F433 T434 R444 P445 G450 Q453 L454 K457 E458 H459 K460 D461 S462 V465 N577	K466 I467 Q468 T469 L470 M475 M479 L483 L492 K504 F507 W512 A513 GLU A515 K518 GLU SER LEU LYS ALA PRO SER PHE ALA GLU PRO L530 E536 F537 F538 D542 A545 M549 I557 C558 L559 E560 S564 P565 K566 P567 R573	K578 K579 K582 R583 I584 N585 S586 A587 F588 V592 K606 I607 R608 E609 W610 H611 Q612 Q615 ILE SER GLY
---	--	---	---	--	---

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.54Å 159.42Å 181.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 3.16 19.95 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.95-3.16) 99.5 (19.95-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.94 (at 3.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.264 , 0.283 0.253 , 0.290	Depositor DCC
R_{free} test set	1268 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 13.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25325 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FLC

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	0.61	8/4207 (0.2%)	0.61	4/5644 (0.1%)
1	B	0.62	1/2615 (0.0%)	0.60	0/3512
All	All	0.62	9/6822 (0.1%)	0.60	4/9156 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	TYR	CD2-CE2	-7.53	1.28	1.39
1	A	183	TYR	CD1-CE1	-7.23	1.28	1.39
1	A	159	VAL	CB-CG2	-7.20	1.37	1.52
1	B	394	GLU	CB-CG	-5.91	1.41	1.52
1	A	183	TYR	CE2-CZ	-5.82	1.30	1.38
1	A	406	TYR	CD2-CE2	-5.56	1.31	1.39
1	A	160	VAL	CB-CG1	-5.17	1.42	1.52
1	A	275	PHE	CE2-CZ	-5.07	1.27	1.37
1	A	87	TYR	CE2-CZ	-5.06	1.31	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	174	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	167	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	A	546	LEU	CB-CG-CD2	-5.28	102.03	111.00

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	4130	0	4151	160	0
1	B	2569	0	2573	73	0
2	A	6	0	8	0	0
2	B	24	0	32	0	0
3	A	13	0	5	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
All	All	6745	0	6769	234	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 17.

All (234) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:LYS:NZ	1:B:172:PHE:CE2	1.88	1.34
1:A:431:ARG:HH21	1:A:431:ARG:CG	1.67	1.06
1:A:161:LEU:HD12	1:A:165:GLU:HG2	1.07	1.06
1:A:431:ARG:HH21	1:A:431:ARG:HG2	1.20	1.05
1:A:98:GLU:HA	1:A:159:VAL:HG12	1.38	1.05
1:A:390:VAL:HG22	1:A:391:TRP:H	1.21	1.01
1:A:161:LEU:CD1	1:A:165:GLU:HG2	1.89	1.01
1:A:247:THR:HG22	1:A:251:LYS:HZ1	1.33	0.94
1:A:174:ARG:HH11	1:A:174:ARG:CG	1.81	0.93
1:A:390:VAL:CG2	1:A:391:TRP:H	1.81	0.93
1:B:217:LYS:O	1:B:219:ILE:N	2.03	0.90
1:B:168:LYS:HZ1	1:B:172:PHE:HE2	0.95	0.87
1:A:431:ARG:NH2	1:A:431:ARG:HG2	1.85	0.87
1:B:151:HIS:ND1	1:B:151:HIS:O	2.07	0.86
1:B:549:MSE:O	1:B:583:ARG:NH1	2.10	0.84
1:B:200:ARG:HB2	1:B:200:ARG:NH1	1.94	0.82
1:A:389:ASN:OD1	1:A:389:ASN:N	2.13	0.81
1:A:247:THR:HG22	1:A:251:LYS:NZ	1.95	0.81
1:B:461:ASP:O	1:B:466:LYS:NZ	2.12	0.81
1:A:470:LEU:HD22	1:A:517:ILE:HD13	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:LYS:NZ	1:B:172:PHE:CZ	2.50	0.79
1:B:256:ASP:OD1	1:B:256:ASP:N	2.12	0.78
1:A:444:ARG:NH1	1:A:449:GLU:OE1	2.16	0.78
1:B:573:ARG:HH11	1:B:573:ARG:HB3	1.48	0.78
1:A:174:ARG:HH11	1:A:174:ARG:HG2	1.47	0.77
1:A:161:LEU:HD12	1:A:165:GLU:CG	2.03	0.77
1:A:340:SER:O	1:A:344:ASN:ND2	2.17	0.77
1:A:449:GLU:O	1:A:453:GLN:HG3	1.85	0.77
1:B:394:GLU:OE2	1:B:425:GLU:HB2	1.84	0.77
1:B:585:ASN:OD1	1:B:608:ARG:NH1	2.20	0.75
1:A:543:GLU:OE1	1:A:544:LYS:N	2.19	0.75
1:A:390:VAL:HG22	1:A:391:TRP:N	2.00	0.74
1:B:394:GLU:OE1	1:B:394:GLU:N	2.21	0.74
1:A:427:ILE:O	1:A:430:ARG:HG3	1.88	0.73
1:B:168:LYS:NZ	1:B:172:PHE:CD2	2.48	0.73
1:A:174:ARG:HH11	1:A:174:ARG:HG3	1.54	0.72
1:B:200:ARG:HB2	1:B:200:ARG:HH11	1.51	0.72
1:B:151:HIS:CE1	1:B:172:PHE:CE2	2.78	0.71
1:A:183:TYR:HB3	1:A:184:PHE:HA	1.73	0.70
1:A:190:ASN:OD1	1:A:190:ASN:N	2.24	0.69
1:A:514:GLU:HA	1:A:517:ILE:HD12	1.74	0.69
1:A:532:ASN:O	1:A:533:LYS:NZ	2.25	0.69
1:A:12:PHE:HZ	1:A:35:LYS:HE2	1.59	0.68
1:A:61:MSE:HG2	1:A:66:ILE:HD11	1.76	0.67
1:B:151:HIS:CE1	1:B:172:PHE:CD2	2.83	0.67
1:B:151:HIS:ND1	1:B:172:PHE:CE2	2.62	0.67
1:A:426:SER:O	1:A:430:ARG:CD	2.42	0.67
1:A:431:ARG:HG3	1:A:431:ARG:HH21	1.59	0.65
1:B:432:LEU:HD23	1:B:445:PHE:HB3	1.77	0.65
1:A:390:VAL:CG2	1:A:391:TRP:N	2.55	0.65
1:A:177:TRP:O	1:A:183:TYR:OH	2.15	0.64
1:A:431:ARG:CG	1:A:431:ARG:NH2	2.39	0.64
1:A:247:THR:O	1:A:251:LYS:NZ	2.30	0.64
1:B:48:PHE:HB2	1:B:50:GLU:HG3	1.78	0.63
1:A:485:LYS:HE2	3:A:702:FLC:HG1	1.80	0.63
1:A:174:ARG:NH1	1:A:174:ARG:CG	2.48	0.63
1:B:394:GLU:CD	1:B:394:GLU:N	2.51	0.63
1:B:512:LEU:O	1:B:512:LEU:HD12	1.99	0.63
1:B:431:ARG:NH1	1:B:560:GLU:OE1	2.31	0.62
1:B:542:ASP:N	1:B:542:ASP:OD1	2.31	0.62
1:B:475:ASN:O	1:B:479:ASN:ND2	2.32	0.62
1:A:426:SER:O	1:A:430:ARG:HD2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:GLU:OE1	1:A:413:ALA:N	2.34	0.61
1:B:168:LYS:CE	1:B:172:PHE:CE2	2.84	0.60
1:A:457:LYS:O	1:A:460:LYS:HG3	2.00	0.60
1:B:151:HIS:CE1	1:B:172:PHE:HE2	2.19	0.60
1:A:174:ARG:HG3	1:A:174:ARG:NH1	2.16	0.59
1:B:215:ASN:OD1	1:B:216:TYR:N	2.36	0.59
1:B:371:VAL:O	1:B:375:ASN:ND2	2.29	0.59
1:B:379:ASP:O	1:B:383:ILE:HG12	2.02	0.58
1:B:327:LYS:HB3	1:B:328:PRO:HD3	1.85	0.58
1:A:408:ASN:ND2	1:A:408:ASN:O	2.34	0.58
1:A:183:TYR:CB	1:A:184:PHE:HA	2.33	0.58
1:A:215:ASN:ND2	1:A:218:LYS:NZ	2.51	0.58
1:A:261:LYS:HE3	1:A:265:GLN:HE21	1.67	0.57
1:A:166:LYS:HB3	1:A:166:LYS:NZ	2.19	0.57
1:B:341:GLU:OE1	1:B:344:ASN:ND2	2.36	0.57
1:A:45:ARG:HG3	1:A:266:LEU:HD21	1.87	0.57
1:A:441:ASN:OD1	1:A:441:ASN:N	2.38	0.57
1:A:183:TYR:HB3	1:A:303:LYS:HZ2	1.70	0.56
1:B:573:ARG:NH1	1:B:573:ARG:HB3	2.20	0.56
1:B:465:VAL:HA	1:B:468:GLN:HG2	1.87	0.56
1:A:371:VAL:HG22	1:A:478:ILE:HD13	1.88	0.55
1:B:391:TRP:H	1:B:391:TRP:HD1	1.54	0.55
1:A:511:GLN:HA	1:A:514:GLU:HG2	1.88	0.55
1:A:166:LYS:C	1:A:167:GLU:CG	2.75	0.55
1:A:133:ASN:OD1	1:A:134:LYS:N	2.40	0.55
1:A:166:LYS:C	1:A:167:GLU:HG2	2.28	0.54
1:A:183:TYR:N	1:A:183:TYR:CD1	2.73	0.54
1:A:174:ARG:HA	1:A:177:TRP:CG	2.43	0.54
1:B:251:LYS:O	1:B:253:ILE:N	2.40	0.54
1:B:582:LYS:O	1:B:586:SER:HB3	2.07	0.54
1:A:191:ASP:OD2	1:A:191:ASP:N	2.39	0.53
3:A:702:FLC:OHB	3:A:702:FLC:OG1	2.24	0.53
1:A:12:PHE:CZ	1:A:35:LYS:HE2	2.41	0.53
1:A:135:TYR:HB3	1:A:166:LYS:HD3	1.91	0.53
1:A:287:LYS:O	1:A:291:ILE:HG12	2.09	0.53
1:A:152:SER:HB3	1:A:172:PHE:CZ	2.44	0.53
1:A:186:HIS:N	1:A:187:PRO:HD3	2.23	0.53
1:A:531:PRO:HD2	1:A:533:LYS:NZ	2.24	0.52
1:A:341:GLU:OE1	1:A:341:GLU:N	2.34	0.52
1:A:143:MSE:HG3	1:A:144:PHE:N	2.24	0.52
1:B:394:GLU:C	1:B:429:LEU:HD12	2.31	0.52
1:A:427:ILE:O	1:A:430:ARG:CG	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:ILE:HD12	1:A:90:ILE:HD12	1.91	0.51
1:B:151:HIS:CE1	1:B:172:PHE:HD2	2.28	0.51
1:A:406:TYR:HD1	1:A:454:LEU:CD1	2.23	0.51
1:B:327:LYS:HG3	1:B:357:LYS:O	2.11	0.51
1:A:158:ILE:HG13	1:A:214:LEU:HD11	1.93	0.51
1:A:516:ASP:N	1:A:516:ASP:OD1	2.43	0.51
1:A:405:LEU:O	1:A:407:ASP:N	2.44	0.50
1:A:436:ASP:OD2	1:A:439:THR:OG1	2.29	0.50
1:A:28:TYR:HB2	1:A:36:PHE:HB2	1.93	0.50
1:A:87:TYR:OH	1:A:256:ASP:HB3	2.11	0.50
1:A:402:LEU:HD23	1:A:402:LEU:O	2.12	0.50
1:A:179:ASP:O	1:A:182:ARG:N	2.45	0.50
1:B:479:ASN:O	1:B:483:ILE:HG12	2.12	0.49
1:A:334:THR:OG1	1:A:335:SER:N	2.45	0.49
1:A:300:ARG:O	1:A:304:ILE:HG13	2.13	0.49
1:A:413:ALA:HB3	1:A:592:VAL:HG11	1.95	0.49
1:A:371:VAL:HG21	1:A:440:PHE:HD1	1.78	0.49
1:A:262:THR:HA	1:A:265:GLN:HB2	1.94	0.49
1:A:388:ASN:OD1	1:A:388:ASN:N	2.45	0.49
1:B:504:LYS:O	1:B:507:PHE:HB2	2.13	0.49
1:A:215:ASN:ND2	1:A:218:LYS:HZ2	2.11	0.48
1:B:391:TRP:N	1:B:391:TRP:CD1	2.80	0.48
1:A:406:TYR:CD1	1:A:454:LEU:HD12	2.49	0.48
1:A:470:LEU:HB2	1:A:517:ILE:HD11	1.96	0.47
1:A:177:TRP:CE3	1:A:300:ARG:NH1	2.81	0.47
1:B:250:LEU:O	1:B:252:ASN:N	2.46	0.47
1:B:256:ASP:O	1:B:257:LEU:HD23	2.14	0.47
1:B:409:SER:HB2	1:B:414:ILE:HD11	1.97	0.47
1:A:50:GLU:HG2	1:A:171:GLN:O	2.15	0.47
1:A:52:PHE:HE2	1:A:293:MSE:HE3	1.80	0.47
1:B:462:SER:O	1:B:466:LYS:HG2	2.14	0.47
1:A:45:ARG:NH1	1:A:269:TYR:CE1	2.83	0.47
1:A:326:LEU:HB3	1:A:327:LYS:H	1.49	0.47
1:A:577:ASN:OD1	1:A:578:LYS:N	2.48	0.47
1:A:577:ASN:OD1	1:A:579:LYS:N	2.36	0.47
1:A:542:ASP:OD1	1:A:545:ALA:HB3	2.15	0.47
1:A:549:MSE:O	1:A:583:ARG:NH1	2.47	0.47
1:B:151:HIS:ND1	1:B:172:PHE:CD2	2.83	0.46
1:A:458:GLU:H	1:A:458:GLU:CD	2.19	0.46
1:A:35:LYS:HG3	1:A:93:LEU:HD13	1.97	0.46
1:A:152:SER:OG	1:A:152:SER:O	2.29	0.46
1:B:330:THR:OG1	1:B:331:LEU:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:ASN:OD1	1:A:579:LYS:HB2	2.16	0.46
1:A:459:HIS:HB3	1:A:462:SER:HB2	1.96	0.46
1:A:143:MSE:HB3	1:A:226:MSE:HG2	1.97	0.46
1:B:413:ALA:HB3	1:B:592:VAL:HG11	1.98	0.46
1:A:261:LYS:HE3	1:A:265:GLN:NE2	2.30	0.46
1:A:587:ALA:O	1:A:590:SER:OG	2.27	0.46
1:A:73:SER:HG	1:A:167:GLU:CD	2.19	0.46
1:A:174:ARG:HG2	1:A:174:ARG:NH1	2.20	0.45
1:A:296:LEU:O	1:A:300:ARG:HG3	2.16	0.45
1:A:184:PHE:HA	1:A:303:LYS:HZ2	1.81	0.45
1:A:215:ASN:ND2	1:A:218:LYS:HZ3	2.15	0.45
1:A:40:LYS:HD3	1:A:82:PHE:HE2	1.81	0.45
1:B:518:LYS:HD3	1:B:518:LYS:HA	1.38	0.45
1:A:543:GLU:HG3	1:A:544:LYS:HD2	1.98	0.45
1:A:70:TYR:O	1:A:73:SER:HB2	2.16	0.45
1:A:11:ARG:HG2	1:A:12:PHE:N	2.29	0.45
1:A:166:LYS:HZ3	1:A:166:LYS:HB3	1.81	0.45
1:A:102:VAL:HG23	1:A:103:ILE:HG23	1.99	0.44
1:A:183:TYR:N	1:A:183:TYR:HD1	2.14	0.44
1:A:170:LYS:HE2	1:A:170:LYS:HB2	1.76	0.44
1:A:228:GLU:O	1:A:232:GLN:HB2	2.17	0.44
1:A:362:SER:O	1:A:485:LYS:NZ	2.50	0.44
1:A:372:LYS:HB2	1:A:372:LYS:HE3	1.78	0.44
1:A:47:LEU:HD12	1:A:89:LEU:HG	1.98	0.44
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.88	0.44
1:A:531:PRO:HD2	1:A:533:LYS:HZ3	1.82	0.44
1:A:479:ASN:O	1:A:482:LYS:HB2	2.18	0.44
1:B:558:CYS:HB3	1:B:607:ILE:HD13	2.00	0.44
1:B:457:LYS:HA	1:B:460:LYS:NZ	2.33	0.44
1:B:504:LYS:HB3	1:B:504:LYS:HE3	1.78	0.43
1:A:517:ILE:O	1:A:519:GLU:N	2.39	0.43
1:A:152:SER:O	1:A:157:ASN:ND2	2.51	0.43
1:A:35:LYS:HG2	1:A:93:LEU:HD22	2.01	0.43
1:B:467:ILE:O	1:B:470:LEU:HB3	2.18	0.43
1:A:385:CYS:HB3	1:A:391:TRP:CZ2	2.54	0.43
1:A:73:SER:OG	1:A:167:GLU:CD	2.52	0.43
1:A:78:ASP:OD1	1:A:79:VAL:N	2.50	0.43
1:A:177:TRP:HZ2	1:A:293:MSE:SE	2.51	0.43
1:B:432:LEU:CD2	1:B:445:PHE:HB3	2.47	0.43
1:A:158:ILE:HA	1:A:167:GLU:O	2.19	0.43
1:A:455:TYR:N	1:A:458:GLU:OE1	2.48	0.42
1:B:538:PHE:CE2	1:B:557:ILE:HG23	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:HIS:HB3	1:A:188:ASN:HD22	1.85	0.42
1:A:84:ASP:O	1:A:85:LYS:HB3	2.19	0.42
1:B:151:HIS:ND1	1:B:172:PHE:HE2	2.13	0.42
1:A:31:ASN:OD1	1:A:31:ASN:N	2.52	0.42
1:B:213:PHE:O	1:B:492:ILE:HG23	2.19	0.42
1:A:467:ILE:HG22	1:A:468:GLN:N	2.34	0.42
1:A:371:VAL:HG21	1:A:440:PHE:CD1	2.54	0.42
1:A:406:TYR:CD1	1:A:454:LEU:CD1	3.02	0.42
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.80	0.42
1:A:457:LYS:HB2	1:A:458:GLU:H	1.71	0.42
1:A:253:ILE:HG23	1:A:257:LEU:HD22	2.01	0.42
1:B:331:LEU:HB3	1:B:346:TRP:CE2	2.55	0.42
1:A:546:LEU:O	1:A:546:LEU:HD12	2.19	0.42
1:A:457:LYS:HB2	1:A:458:GLU:OE1	2.20	0.41
1:B:406:TYR:HD1	1:B:454:LEU:HB2	1.85	0.41
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.28	0.41
1:A:390:VAL:O	1:A:391:TRP:C	2.59	0.41
1:A:510:PHE:O	1:A:514:GLU:HB3	2.20	0.41
1:B:48:PHE:C	1:B:48:PHE:CD1	2.94	0.41
1:A:154:HIS:H	1:A:157:ASN:HB2	1.85	0.41
1:A:596:ARG:NH1	1:A:598:ASP:OD2	2.53	0.41
1:A:98:GLU:OE2	1:A:156:GLY:O	2.38	0.41
1:A:54:GLY:HA2	1:A:76:CYS:HB2	2.02	0.41
1:A:150:ALA:HB1	1:A:168:LYS:NZ	2.36	0.41
1:B:609:GLU:HA	1:B:612:GLN:HG2	2.01	0.41
1:A:43:ASP:OD1	1:A:44:PRO:HD2	2.21	0.41
1:B:577:ASN:OD1	1:B:579:LYS:HG3	2.21	0.41
1:B:415:HIS:HD2	1:B:444:ARG:HD3	1.85	0.41
1:B:450:GLY:O	1:B:453:GLN:HB2	2.21	0.41
1:A:160:VAL:HG12	1:A:161:LEU:O	2.21	0.41
1:A:145:SER:OG	1:A:168:LYS:HD2	2.21	0.41
1:A:504:LYS:HB3	1:A:504:LYS:HE3	1.93	0.41
1:A:606:LYS:O	1:A:609:GLU:HG2	2.21	0.41
1:B:337:THR:HG21	1:B:341:GLU:HG2	2.03	0.41
1:B:157:ASN:HD22	1:B:157:ASN:HA	1.56	0.41
1:A:339:PHE:O	1:A:343:ILE:HG12	2.21	0.41
1:B:564:SER:HA	1:B:565:PRO:HD3	1.94	0.41
1:B:454:LEU:N	1:B:454:LEU:HD23	2.35	0.40
1:A:341:GLU:O	1:A:344:ASN:HB2	2.22	0.40
1:B:606:LYS:HE2	1:B:610:TRP:CZ2	2.57	0.40
1:A:436:ASP:HA	1:A:437:PRO:HD3	1.90	0.40
1:A:343:ILE:HD12	1:A:477:ILE:HD13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:SER:O	1:A:430:ARG:CG	2.69	0.40
1:A:242:LEU:HD13	1:A:298:GLU:HB2	2.03	0.40
1:B:422:TYR:OH	1:B:545:ALA:HB1	2.21	0.40
1:B:363:ASN:N	1:B:364:PRO:HD2	2.35	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	498/626 (80%)	465 (93%)	26 (5%)	7 (1%)	16	64
1	B	293/626 (47%)	267 (91%)	22 (8%)	4 (1%)	16	64
All	All	791/1252 (63%)	732 (92%)	48 (6%)	11 (1%)	16	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	187	PRO
1	A	390	VAL
1	B	251	LYS
1	A	211	ASP
1	A	406	TYR
1	A	455	TYR
1	B	252	ASN
1	A	457	LYS
1	B	567	PRO
1	B	254	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	446/526 (85%)	389 (87%)	57 (13%)	6	27
1	B	278/526 (53%)	236 (85%)	42 (15%)	4	19
All	All	724/1052 (69%)	625 (86%)	99 (14%)	5	24

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	31	ASN
1	A	35	LYS
1	A	39	LYS
1	A	45	ARG
1	A	46	GLU
1	A	49	THR
1	A	68	GLU
1	A	93	LEU
1	A	95	SER
1	A	143	MSE
1	A	152	SER
1	A	164	GLU
1	A	166	LYS
1	A	169	SER
1	A	171	GLN
1	A	174	ARG
1	A	177	TRP
1	A	182	ARG
1	A	183	TYR
1	A	186	HIS
1	A	190	ASN
1	A	191	ASP
1	A	210	LYS
1	A	229	LYS
1	A	273	ASP
1	A	282	THR
1	A	283	GLU
1	A	334	THR
1	A	337	THR
1	A	338	SER
1	A	340	SER
1	A	348	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	ASP
1	A	376	LEU
1	A	383	ILE
1	A	388	ASN
1	A	389	ASN
1	A	390	VAL
1	A	391	TRP
1	A	408	ASN
1	A	412	GLU
1	A	414	ILE
1	A	426	SER
1	A	430	ARG
1	A	431	ARG
1	A	445	PHE
1	A	460	LYS
1	A	467	ILE
1	A	475	ASN
1	A	514	GLU
1	A	516	ASP
1	A	519	GLU
1	A	541	ILE
1	A	543	GLU
1	A	570	LEU
1	A	579	LYS
1	B	49	THR
1	B	51	LEU
1	B	52	PHE
1	B	55	LEU
1	B	153	VAL
1	B	157	ASN
1	B	161	LEU
1	B	166	LYS
1	B	170	LYS
1	B	211	ASP
1	B	217	LYS
1	B	250	LEU
1	B	251	LYS
1	B	253	ILE
1	B	254	PRO
1	B	256	ASP
1	B	329	LEU
1	B	336	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	340	SER
1	B	344	ASN
1	B	349	ILE
1	B	361	ASP
1	B	365	ILE
1	B	386	GLU
1	B	390	VAL
1	B	391	TRP
1	B	394	GLU
1	B	403	PHE
1	B	408	ASN
1	B	412	GLU
1	B	434	THR
1	B	458	GLU
1	B	530	LEU
1	B	536	GLU
1	B	542	ASP
1	B	573	ARG
1	B	579	LYS
1	B	582	LYS
1	B	583	ARG
1	B	586	SER
1	B	588	PHE
1	B	615	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	B	157	ASN
1	B	479	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	701	-	5,5,5	0.35	0	5,5,5	0.23	0
3	FLC	A	702	-	5,12,12	7.91	4 (80%)	7,17,17	3.23	3 (42%)
2	GOL	B	701	-	5,5,5	0.31	0	5,5,5	0.32	0
2	GOL	B	702	-	5,5,5	0.32	0	5,5,5	0.20	0
2	GOL	B	703	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	B	704	-	5,5,5	0.33	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	701	-	-	0/4/4/4	0/0/0/0
3	FLC	A	702	-	-	0/6/16/16	0/0/0/0
2	GOL	B	701	-	-	0/4/4/4	0/0/0/0
2	GOL	B	702	-	-	0/4/4/4	0/0/0/0
2	GOL	B	703	-	-	0/4/4/4	0/0/0/0
2	GOL	B	704	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FLC	CA-CAC	15.93	1.59	1.49
3	A	702	FLC	CG-CB	-5.22	1.46	1.54
3	A	702	FLC	OHB-CB	4.02	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FLC	CA-CB	3.91	1.61	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FLC	CB-CG-CGC	-5.84	106.28	115.01
3	A	702	FLC	CG-CB-CBC	-5.52	100.05	111.21
3	A	702	FLC	CG-CB-CA	2.30	115.11	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	515/626 (82%)	-0.30	0 100 100	9, 37, 72, 105	0
1	B	319/626 (50%)	-0.22	0 100 100	15, 47, 80, 92	0
All	All	834/1252 (66%)	-0.27	0 100 100	9, 41, 75, 105	0

There are no RSRZ outliers to report.

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	701	6/6	0.33	3.14	39,48,56,59	0
3	FLC	A	702	13/13	0.22	0.96	28,36,60,67	0
2	GOL	B	701	6/6	0.26	-0.21	21,38,43,59	0
2	GOL	B	703	6/6	0.41	-	35,58,65,66	0
2	GOL	B	704	6/6	0.28	-	49,52,73,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	702	6/6	0.24	-	36,51,55,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.